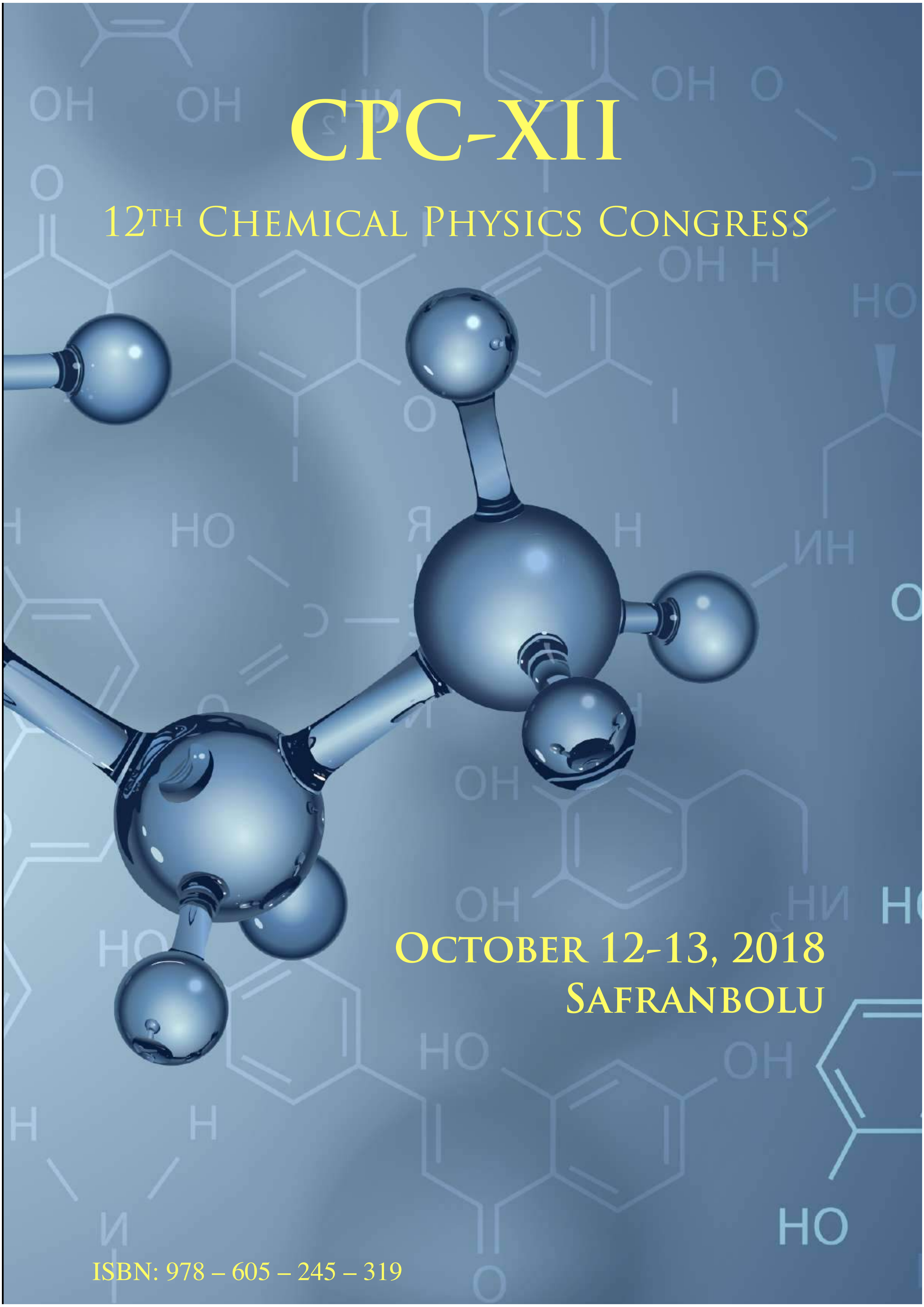

CPC-XII

12TH CHEMICAL PHYSICS CONGRESS

OCTOBER 12-13, 2018
SAFRANBOLU

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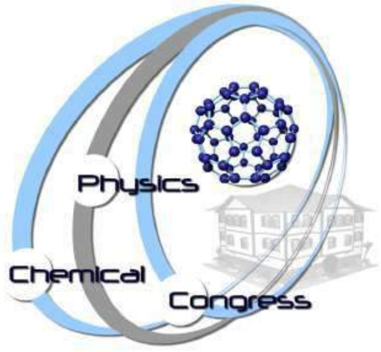

WELCOME

Dear colleagues, fellow scientists, and friends,

It is our great pleasure to welcome you to the 12th of the biannually held Chemical Physics Congress, CPC-XII. The congress will be held on October 12–13, 2018 in Safranbolu – Turkey, a UNESCO world heritage village.

The scientific program will feature four plenary lectures delivered by George C. Schatz, Yves Leterrier, Helmut Schwarz, and Peter B. Armentrout. There will be 19 invited talks and 15 short oral communications. The number of poster presentations is 49. CPC–XII will cover many different topics including but not limited to, surface science, spectroscopy, catalysis, theory, statistical mechanics, and computation.

We would like to express our sincerest thanks to all of our participants to make this wonderful event happen and to all of our sponsors, particularly Gaussian Inc. for their generous financial support. We look forward to welcoming you in Safranbolu for science, fruitful discussions, and a little 'bite' of social activities.

Sincerely,

Nevin Aytemiz – Murat Kılıç – Yavuz Dede
October 2018 Safranbolu

CPC-XII ORGANIZING COMMITTEE

Nevin Aytemiz	Karabük University, Karabük – Turkey	nevinaytemiz@gmail.com
Murat Kılıç	EPFL, Lausanne – Switzerland	muratmkilic@gmail.com
Yavuz Dede	Gazi University, Ankara – Turkey	labydd@gmail.com

CPCS SCIENTIFIC COMMITTEE

(alphabetical order according to the last name)

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Zekiye Çınar Yıldız Technical University, İstanbul – Turkey
Şefik Süzer Bilkent University, Ankara – Turkey
Ersin Yurtsever Koç University, İstanbul – Turkey
Mine Yurtsever İstanbul Technical University, İstanbul – Turkey

‘Some reminiscences on the history of Chemical Physics in Turkey’ by Ersin Yurtsever

In my opinion chemical physics in Turkey started in 1968 when three former students of Oktay Sinanoğlu started a graduate school of ‘Theoretical Chemistry’ in Orta Doğu Teknik Üniversitesi. Even though this adventure did not last very long, it introduced new concepts to Turkish Science. The regulations for docentship has ‘theoretical chemistry’ as one of the formally accepted areas of basic sciences even though it has become ‘computational chemistry’ nowadays and we still do not have ‘chemical physics’ in that list.

The history of experimental studies of fundamental process in Turkey is also not very old, mostly due to the high costs of the setups. However, theory could not survive without the experiments and vice versa. So with the idea of bringing experimentalists and theoreticians in a forum together, we started a series of conferences. This first ‘experimental’ one was a session in 1984 in ODTÜ and then in Boğaziçi in 1986. The first session had 4-5 talks with probably 10 people attending, some for simply curiosity. Nowadays, it is nice to see that CPC conferences attract reasonable crowds with well-known names from abroad and young scientist who are doing exciting work.

KEYNOTE SPEAKERS

(alphabetical order according to the last name)

Peter Armentrout, University of Utah, Utah – United States
Yves Leterrier, EPFL, Lausanne – Switzerland
George Schatz, Northwestern University, Illinois – United States
Helmut Schwarz, Technical University of Berlin, Berlin – Germany

INVITED SPEAKERS

(alphabetical order according to the last name)

Şule Atahan Evrenk TOBB University of Economics & Technology, Ankara – Turkey
Canan Atılgan Sabancı University, İstanbul – Turkey
Viktorya Aviyente Boğaziçi University, İstanbul – Turkey
Umut Aydemir Koç University, İstanbul – Turkey
Turgut Baştuğ Hacettepe University, Ankara – Turkey
Uğur Bozkaya Hacettepe University, Ankara – Turkey
Niyazi Bulut Fırat University, Elazığ – Turkey
Şaron Çatak Boğaziçi University, İstanbul – Turkey
Nihan Çelebi Ölçüm Yeditepe University, İstanbul – Turkey
Sondan Feyiz Durukanoğlu Kadir Has University, İstanbul – Turkey
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Emrah Özensoy Bilkent University, Ankara – Turkey
Ulrike Salzner Bilkent University, Ankara – Turkey
Şefik Süzer Bilkent University, Ankara – Turkey
Alper Uzun Koç University, İstanbul – Turkey
Mine Yurtsever İstanbul Technical University, İstanbul – Turkey
Ersin Yurtsever Koç University, İstanbul – Turkey

CPC–XII: 12th Chemical Physics Congress

KEYNOTE LECTURES

KL–1

SERS and Theory

George C. Schatz

Northwestern University, Department of Chemistry, Evanston, IL – United States

Silver and gold nanoparticles have a history that dates to the Roman Empire and before, as well as detailed work by Michael Faraday in the 1850s. However these particles have been given new directions in the last 40 years through a number of advances in nanoscience, and especially by the discovery of surface enhanced Raman spectroscopy (SERS) in the 1970s. This talk will provide an overview of these advances, including the development of SERS substrates with extremely high enhancement factors, the discovery of single-molecule SERS, and new developments in tip enhanced Raman spectroscopy (TERS). An emphasis in this talk will be on the use of theory to understand the optical properties of plasmonic materials, the SERS enhancement, and the coupling of TERS to single molecule electrochemistry.

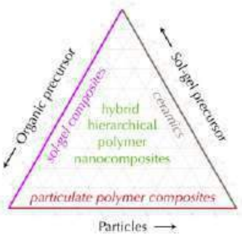
KL–2

Hybrid Hierarchical Polymer Nanocomposites

Luca Mueller, Feyza Karasu, Yves Leterrier

Ecole Polytechnique Fédérale de Lausanne (EPFL), Laboratory for Processing of Advanced Composites (LPAC), Lausanne – Switzerland

Novel integrative and bio-inspired synthetic strategies have emerged in the past two decades as alternatives to conventional polymer processing and soft chemistry routes developed in the 1980s. The presentation will give an overview of the activities carried out at the EPFL to produce hybrid organic-inorganic architectures hierarchically organized in terms of structure and functions. These materials are based on organic and organometallic precursors and preformed nanoparticles, and dual-cure condensation and photopolymerization processes [1,2]. Selected components include acrylated and epoxidized oligomers, tetraethyl orthosilicate and silica particles, and organosilanes as coupling agents. The research explores the process-structure-property relations within the corresponding ternary phase diagram (Fig. 1) and highlights the role of individual components and interfacial interactions from the analysis of suspension rheology [3]. The dynamics of network formation is investigated using novel photo-hyphenated methods such as photo-rheology and photo-calorimetry [4]. Solidified materials are characterized using an array of thermomechanical methods. Applications examples include diffusion barrier coatings [5] and bio-inspired, functional surfaces such as 'moth-eye' antireflective coatings [6] and wear resistant self-cleaning 'lotus' surfaces (Fig. 2, [7]).



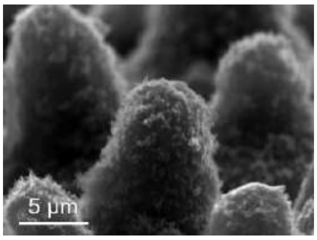


Figure 1: Ternary phase diagram for dual-cure, hybrid hierarchical polymer nano-composites
Figure 2: Scanning electron micrograph of a synthetic nanocomposite lotus surface produced using an ambient UV printing process. The surface is wear-resistant and superhydrophobic

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KL–3

A Mass Spectrometry and Theoretical Chemistry in Service of Catalysis Research: A Ménage-á-Trois at Its Best

Helmut Schwarz

Technische Universität Berlin, Institut für Chemie, Berlin – Germany

The ultimate goal in heterogeneous catalysis is to make use of each and every atom of supported (metal) catalysts, i.e. in the extreme to perform single-atom catalysis (SAC). While this arduous task constitutes a non-trivial, if not daunting challenge in 'real-life' chemistry, in the gas phase SAC can be achieved in a rather straightforward manner by conducting experiments with mass-selected species under (near) single-collision conditions. These mass spectrometry-based studies on isolated reactants, when complemented by state-of-the-art computational and spectroscopic work, provide an ideal arena for probing the energetics and kinetics of a chemical process in an unperturbed environment at a strictly molecular level without being obscured by ill-defined side effects. Thus, the concept of SAC can be explored or, more generally, the mechanisms of reactions and the active parts of single-site catalysts, the so-called 'aristocratic' atoms, can be identified.
Examples discussed include: (i) The room-temperature, cluster-oxide mediated redox reactions of the CO/N_2O couple which, arguably constitute one of the most prominent oxidation processes, and (ii) novel metal-mediated C–H bond activation and C=C coupling of methane, which are regarded as one of the holy grails in chemistry.

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KL–4

Reactivity of Lanthanides and Actinides: Chemi-ionization, Thermochemistry, Mechanisms, and Spin-orbit Effects

Peter B. Armentrout, R. M. Cox, M. Demireva

University of Utah, Department of Chemistry, Salt Lake City, UT – United States

The US Air Force is interested in avoiding an effect called scintillation that can disrupt satellite communication for minutes at a time. Scintillation is caused by inhomogeneities in the plasma density in the ionosphere. Artificially induced plasmas can mediate this and can be formed by a chemi-ionization reaction in which formation of a strong bond is sufficiently exothermic to induce ionization (creating a cation and electron). Several early transition metals and several lanthanides are known to undergo this process by reaction of the metal atom with an oxygen atom (abundant in the ionosphere), $M + O \rightarrow MO^+ + e^-$. Early atmospheric tests using samarium (Sm) showed differences with predicted behavior, indicating that the thermochemistry was not known with sufficient accuracy. This talk will outline our recent guided ion beam tandem mass spectrometry (GIBMS) results on the thermochemistry of samarium oxide. These explorations also reveal interesting diabatic behavior that characterizes whether electrons are free to move freely between f orbitals and valence (s and d) orbitals used in bonding during reactions of lanthanides. This ability pertains to the prospects of using lanthanides as powerful catalytic reagents. Naturally, the exploration of such heavy metals means that spin-orbit interactions become important, a lesson that we have explored quantitatively by examining chemistry of the actinide thorium. In particular, the chemistry of Th^+ with water has been examined both experimentally using GIBMS as well as theoretically. Although studied previously by others, the ability to examine the kinetic energy dependence of these reactions provides much more complete and quantitative information about the mechanisms and thermodynamics of such processes.

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CPC–XII: 12th Chemical Physics Congress

INVITED LECTURES

IL–1

X-Ray Photoelelctron Spectroscopy, a Chemical Tool for Electrochemical Analyses of Potential Developments at Liquid/Solid Interfaces: Past, Present and Future

Şefik Süzer

Bilkent University, Department of Chemistry, Ankara – Turkey

Charge distribution, storage and movement in solutions and soft-matter are of paramount importance for understanding and intelligent use of various electrochemical concepts towards advanced applications in energy, chemical, biochemical, microfluidics and sensing. Over the last three decades the vast research efforts using advanced measurement, computational and simulation techniques have changed the old concept of electroneutrality assumed, and most of the time enforced, to be obeyed in many physicochemical processes taking place in solution surfaces or in pores of solid materials. Being a chemically sensitive and quantitative surface analysis technique, x-ray photoelectron spectroscopy (XPS) has been the pivotal method to extract information about distribution of cations and anions on various surface structures, once difficulties in handling liquids had been overcome through multiple advancements in experimental techniques. The pioneering XPS investigation of ion enrichment on surfaces of viscous liquids by H. Siegbahn,[1] was later successfully extended to aqueous solutions in the form of micro-droplets, using synchrotron based photoemission spectroscopy by Faubel and coworkers.[2] In parallel, developments in ambient pressure XPS have enabled investigation of a large variety of critical materials and chemical processes.[3] All of these giant leaps and developments have also been successfully supported and guided by extensive molecular dynamics simulations. Nonvolatile room temperature ionic liquid (RTIL) electrolytes have allowed us and others to utilize lab-based XPS instruments for investigating various electrochemical processes under ultrahigh vacuum conditions, without the need for extensive pumping techniques nor synchrotron facilities. In this contribution, we report on using a similar multi-layered graphene as the top electrode and utilize XPS to monitor in-situ; (i) the changes in the anion/cation intensity ratio under applied electric fields, and (ii) the electrical potential developments on different surface structures, which are derived from the shifts in the binding energies of the corresponding atomic core levels in a chemically resolved fashion.[4-10]

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IL–2

A Tale of Two Catalysts: Bulk Oxygen Vacancy Driven Catalysis on Perovskite Surfaces and Imaging Sulfur Poisoning of Precious Metal Catalysts at the Nanometer Scale with Chemical Definition

Emrah Özensoy

Bilkent University, Department of Chemistry, Ankara – Turkey

In the first part of my presentation I will talk about a simple and a reproducible synthetic protocol to synthesize hybrid perovskites with a nominal stoichiometry of $LaCo_xMn_{1-x}O_3$ (x = 0.1-0.9), whose bulk B-site stoichiometry, surface/bulk B-site oxidation states, and bulk oxygen vacancy population can be controlled in a gradual manner. Structural and functional properties of these materials were investigated with: XRD, BET, ICP-MS, XPS, TEM, ex-situ and in-situ XANES, *in-situ* FTIR and TPD. An efficient methodology was presented to estimate the bulk stoichiometry and the bulk oxygen deficiency of the hybrid perovskites by combining average bulk-oxidation state information provided by XANES and bulk A-site and B-site atomic ratios measured in ICP-MS. Here, we demonstrate that these bulk-oxygen vacancies have a strong influence on the redox activity of the hybrid perovskites allowing them to efficiently switch between high and low B-site oxidation states in a reversible fashion under relatively moderate redox conditions without requiring elevated temperatures for regeneration, unlike $LaCoO_3$ and $LaMnO_3$ benchmark systems. It is likely that this is accomplished by the diffusion of bulk oxygen vacancies to the surface which eventually governs the surface redox reactivity. In the second part of my talk, I will talk about our recent Scanning Near Optical Field Microscopy (SNOM) studies on a 2D (planar) model catalyst system comprised of iridium nanoparticles supported on a TiO_2 thin-film grown on a single crystal Si wafer support material. Unlike conventional infrared microscopy, where the state-of-the-art spatial resolution is *ca.* 1 μm, we will show that SNOM imaging allows a spatial resolution of *ca.* 20 nm. Using this ultra-high spatial resolution offered by SNOM (NanoIR microscopy), we will demonstrate that, not only can we differentiate different SO_x species (e.g. sulfates and sulfites with dissimilar surface orientations) located on iridium precious metal nanoparticles versus TiO_2 support material, but we can also identify and even map these different SO_x species poisoning the catalyst surface with nanometer scale resolution.

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IL–3

Machine Learning for the Prediction of Reorganization Energy for P–type Molecular Organic Semiconductors

Şule Atahan Evrenk[1], **Seçil Usta**[2], **F. Betül Atalay**[2]

[1]TOBB University of Economics & Technology, Faculty of Medicine, Ankara – Turkey
[2]TOBB University of Economics & Technology, Department of Computer Engineering, Ankara – Turkey

Organic Semiconductors (OSCs) have potential for many electronic and photovoltaic applications since they are solution processable and compatible with plastics. Moreover, the vast chemical space presents an immense opportunity for the design of novel functional materials with improved stability and performance. High-throughput computational screening provides a cost-affective and facile avenue for the exploration of this chemical space. For the preliminary screening, predictive models based on a simple representation of molecular structure are crucial. In this research, we focused on the reorganization energy (RE), an important charge transfer parameter, in order to adapt it as such a preliminary screening parameter.

Usual $intra$molecular RE calculation involves full geometry optimization of the neutral and ionic state of the molecule. Although trivial in small scale, these optimizations are expensive for large-scale screening. Our approach brings methods from cheminformatics and quantum chemistry together to predict the RE from molecular structure only. To this end, we built a compound library, which consists of 5712 conjugated backbones; the largest library to date dedicated to the study of the RE. We started with benzene, thiophene, furan, pyrrole, pyridine, pyridazine and cyclopentadiene as building blocks represented as SMILES strings. These building blocks were fused together to obtain extended conjugated backbones up to five rings using SMARTS reaction rules. The initial geometries were obtained with MMFF94 force field. The gas phase RE values were calculated at the density functional theory level with a double zeta basis set with polarization. The RE values ranging from 80 to 480 meV were then used as the target values for models built based on two different representations of the molecules: i) SMILES-based molecular signatures ii) Geometry-based molecular transforms. The kernel ridge regression (KRR) models showed promise with the root-mean-squared-error of 20 meV for the signature and 22 meV for the molecular transform descriptors. The neural networks present a similar performance with the root-mean-squared-error of 22 meV when the molecular signature descriptors were used. The five-fold cross-validated learning curve of the KRR model converges to an error of 20 meV, asymptotically. This study indicates that a machine-learning approach might enable the use of the RE as a parameter for the preliminary screening for the best candidate structures in large OSC compound libraries.

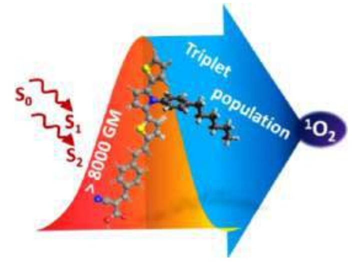
IL–4

Photophysical Properties of Novel Two-photon Absorbing Dyes: Possible Use for Singlet Oxygen Generation

Özlem Şengül[1], Marco Marazzi[2], Antonio Monari[2], Şaron Çatak

[1]Boğaziçi University, Chemistry Department, İstanbul – Turkey
[2]Université de Lorraine and CNRS, LPCT, Nancy – France

Herein, we assess the nonlinear absorption properties and the photophysical profile and behavior of two recently synthesized polythiophenebased dyes. In particular, using high-level state-of-the-art molecular modeling methodologies, we clearly underline the remarkable two-photon absorption (TPA) cross-section. Furthermore, the possible pathways leading to the intersystem crossing and triplet manifold population are investigated by considering the energy difference between the relevant triplet and singlet states on the potential energy surfaces as the key critical points. The spin-orbit coupling is also assessed, and the results globally point to a possible, albeit probably slow, intersystem crossing that could allow the use of the two dyes as singlet oxygen photosensitizers, for instance in photodynamic therapy, owing to their high TPA cross-sections.



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IL–5

Anionic Clusters in Cryogenic Conditions

Ersin Yurtsever

Koç University, Chemistry Department, İstanbul - Turkey

Recently there were several experiments where anionic hydrogen [1] and nitrogen [2] clusters were obtained in liquid helium droplets. The mass spectrometric analysis of both these clusters showed that certain size clusters had relatively high abundances similar to magic sizes. In both cases, clusters with odd number of atoms had much higher abundances/stabilities suggesting a core structure of an odd number of atoms and relatively neutral H_2/N_2 surrounding these cores.

For hydrogen clusters, this core must be a H^- anion. We developed different force fields for the interaction between H^- and H_2 and with these interaction potentials we carried out path-integral molecular dynamics simulations at 1 K. We observed [3] magic numbers at various sizes in agreements with the experimental observations.

In case of nitrogen clusters, azide anion $N_3{}^-$ was the most likely core as it is a very stable anion. We tried to generate force field for N_2 – $N_3{}^-$ interaction; however, a number of different interaction potential types could not even reproduce the structure of $N_5{}^-$. In that case, we tried to generate a quantum mechanical growth mechanism. Starting with $N_5{}^-$, we optimized geometries of $N_{2n+3}{}^-$ where $1 \leq n \leq 9$ with several dispersion-corrected DFT and post-HF methods. For these sizes a two-shell growth model was obtained [4] which supported the proposed azide chromofore model and reasonably agrees with the experiments.

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IL–6

Novel Methods for Increasing the Efficiency of Thermoelectric Materials

Umut Aydemir

Koç University, Department of Chemistry, İstanbul – Turkey
Koç University Akkim Boron-Based Materials and High Technology Chemicals Research and Application Center, İstanbul – Turkey

Globally, two-thirds of the energy produced is lost as waste heat. Among renewable energy sources, thermoelectricity stands for a possible alternative that could not only allow for waste-heat energy harvesting but could also replace compression-based refrigerators [1]. This versatile technology directly converts heat into electricity and vice-versa. Being vibration- and noise-free, reliable, scalable, and without hazardous emissions, solid-state thermoelectric generators can be considered as a clean and sustainable energy source. The thermoelectric efficiency of a given material is quantified through the dimensionless thermoelectric figure of merit, zT, defined as zT = α^2T / $\rho\kappa$, where T is the absolute temperature, α is the thermopower (or Seebeck coefficient), is the electrical resistivity and ρ is the total thermal conductivity which is the sum of the lattice thermal conductivity, κ_L, and the electronic thermal conductivity, κ_E, in non-magnetic materials.

With promising novel structure types and compounds being reported on a frequent basis, Zintl phases represent an important and incredibly diverse new class of thermoelectrics. For the Zintl phase of $Ca_9Zn_{4+x}Sb_9$ [2], despite the complexity of multiple defect types and uncertain defect concentrations, the full range of thermodynamically accessible defects can be explored using "*phase boundary mapping*"' within an isothermal section of the Ca-Zn-Sb ternary phase diagram. Such an equilibrium phase diagram provides the synthesis conditions required to achieve the full range of thermodynamically possible intrinsic defect concentrations to achieve appropriate doping. Demonstrating this principle, optimally doped $Ca_9Zn_{4+x}Sb_9$ containing inexpensive elements can now be produced with a high zT of 1.1 at 875 K, which is one of the highest value among inexpensive p-type thermoelectric without ion conducting.

Microstructure engineering is an effective strategy to reduce κ_L and increase zT . Through a new process based on "*melt-centrifugation*" to squeeze out excess eutectic liquid, microstructure modulation is realized to manipulate the formation of dislocations and clean grain boundaries, resulting in a porous network with a platelet structure in $(Bi,Sb)_2Te_3$ alloys [3]. In this way, phonon transport is strongly disrupted by a combination of porosity, pore surfaces/junctions, grain boundaries, and lattice dislocations. These collectively result in around 60 % reduction of κ_L compared to zone melted ingot, while the charge carriers remain relatively mobile across the liquid-fused grains.

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IL–7

Bionanodesign: Computational Bionanotechnology

Ersin Emre Ören[1,2]

[1]TOBB University of Economics and Technology, Department of Biomedical Engineering,
Bionanodesign Laboratory, Ankara – Turkey
[2]TOBB University of Economics and Technology, Department of Materials Science and
Nanotechnology Engineering, Ankara – Turkey

The realization of nanoscale devices largely depends on our ability to control and manipulate interfacial interactions and thus understanding the mechanisms of surface/interface instabilities and the nature of bio-inorganic interfaces. In this talk, first, the formulation of the dynamics of curved surfaces/interfaces under external forces will be discussed along with its application to design heteroepitaxially grown quantum dots. Quantum dots (QDs) have discrete energy levels thus a well-defined band gap, which may be engineered by controlling their size and morphology. These unique features, plus dislocation-free availability via Stranski Krastanov growth, make QDs promising candidates for various novel optoelectronic devices. Our simulations demonstrated the interplay between the stable QDs and the material properties (e.g., crystallographic orientation and initial thickness of the film, diffusion and surface stiffness anisotropies, surface and interfacial energies, wetting contact angle and mismatch/external stresses). In the second part, the molecular biomimetic approach for the design and utilization of multifunctional molecular systems will be discussed. Here, we describe lessons from biology with examples of DNA, RNA or protein-mediated functional biological materials, explain how novel peptides can be designed with specific affinity to inorganic solids using molecular dynamics and bioinformatics approaches and give examples of their potential utilizations in technology and medicine.

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IL–8

Reactive Scattering Calculations for Astrophysical Importance of O^+ + HD Collisions

Duygu Çimenoğlu Uludağ[1], **Niyazi Bulut**[2], **Octavio Roncero**[3], **François Lique**[4]

[1]Turkish Airlines, Istanbul – Turkey
[2]Fırat University, Department of Physics, Elazığ – Turkey
[3]Instituto de Fisica Fundamental, Department of Atomic, Molecular & Cluster Physics, Madrid – Spain
[4]CNRS–Université du Havre, Laboratoire Ondes et Milieux complexes, Le Havre – France

In space, deuterated species are surprisingly highly abundant. Following the recent discovery of OH^+, we are studying the possible formation of the OD^+ molecule in the interstellar medium. New quantum reactive scattering calculations for the O^+ + HD collisions have been carried out to obtain state-to-state cross sections and rate constants for the title system by using an accurate wave packet approach [1-3] using the doublet and quartet ground H_2O^+ electronic potential energy surfaces correlating to the open shell reactants. Calculations were performed for collision energies in the range of 1 meV to 0.7 eV and for different initial rotational excitation of the reagent molecules. This kind of calculations can provide us a detailed information about atom diatomic molecular collisions.

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IL–9

TDDFT Analysis of Intramolecular Singlet Fission in Biradicals

Ulrike Salzner

Bilkent University, Department of Chemistry, Ankara – Turkey

Singlet fission[1] is a process during which absorption of a single photon creates two triplet excited states on two adjacent chromophores. It was first observed in 1965 in anthracene crystals[2] and in 1989 in a conducting polymer.[3] Intramolecular singlet fission with low yield has been observed in carotenes[4] and its mechanism is poorly understood. It is generally believed that singlet fission proceeds via a singlet excitation on one of the chromophores, followed by charge transfer of the excited electron to the other chromophore.[5] Singlet-coupled triplet pairs form when both chromophores relax to their lower-lying triplet states. The triplet pairs eventually dissociate. The energetic requirement for singlet fission is therefore that the first allowed singlet excited state of the system has at least twice the energy of the first triplet states of the individual chromophores.[6] Further requirements apply that prevent triplet pair annihilation. To analyze the fission probability, most theoretical studies consider the two chromophores as diabatic states and analyse the coupling integrals between them. Here an alternative route is followed that investigates the nature of the adiabatic excited state of the entire system with time-dependent density functional theory. These calculations reveal that for biradicals, a direct (coherent) intramolecular singlet fission mechanism is possible which involves the partial exchange of an α–electron on one chromophore with a β–electro on the other in the first excited state without net charge transfer so that the first excited state has partial singlet-fission character.

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IL–10

An Efficient Analytic Gradients Suite for High-Level Density-Fitted Coupled-Cluster and Perturbation Theories: The DFOCC Module

Uğur Bozkaya

Hacettepe University, Chemistry Department, Ankara – Turkey

Coupled-cluster (CC) methods have proven to be highly reliable for the theoretical estimation of molecular properties. Therefore, high-level coupled-cluster methods are referred as the ‘gold standard’ of computational chemistry. Analytic gradient methods greatly facilitate the location of stationary points on potential energy surfaces and enable the computation of one-electron properties. For these reasons, CC analytic gradients have significant importance in modern computational chemistry. Tensor decompositions of the four-index electron repulsion integrals (ERIs) have been of great interest in modern computational chemistry. One of the popular approximations is density fitting (DF), which is also known as the resolution of the identity (RI). In the DF approach the four-index ERIs are expressed in terms of three-index tensors. It has been demonstrated that the DF approach is very helpful for the efficient evaluation of analytic gradients for the electron correlation methods [1-4]. In this study, we present an efficient analytic gradient suite, the DFOCC module, for the high-level CC and perturbation theories with the density-fitting approximation.

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Acknowledgment This study has been supported by the Scientific and Technological Research Council of Turkey (TUBITAK-114Z786) and the European Cooperation in Science and Technology (CM1405).

IL–11

Building Block Approach for the Preparation of Cyanide-based Chromophore-water Oxidation Catalyst Assemblies

Ferdi Karadaş

Bilkent University, Department of Chemistry, Ankara – Turkey

Cyanide-based assemblies have been investigated in several fields including gas capture and separation, magnetism, and electrochemistry.[1] Recently, cyanide chemistry has also been utilized to construct robust and efficient electrocatalysts for water oxidation.[2] Herein this talk, a novel synthetic approach to covalently coordinate several different chromophores to cyanide-based extended frameworks to prepare chromophore-catalyst assemblies for light-driven water oxidation.

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IL–12

Tuning the Performance of Supported Metal Catalysts with Ionic Liquid Coatings: Nanoparticles to Single-Sites

Alper Uzun

Koç University, Istanbul – Turkey

Controlling the product selectivity is one of the key challenges in heterogeneous catalysis. Modifying the surface characteristics of supports, varying metal nanoparticle size, incorporating promoters or adding a second or third metal offer opportunities for adjusting the electronic environment over the active sites, which in turn controls the catalytic performance. Another approach in this regard is to coat the surface of a solid catalyst with an ionic liquid (IL) layer. In this talk, some of the recent results obtained in our research group by coating supported metal catalysts with ILs will be presented. First, an example on an ordinary commercial supported nickel catalyst will be illustrated. Detailed characterization complemented by density functional theory calculations indicated that an alkylimidazolium type IL coating donates electrons to the active metal sites, making them more selective for partial hydrogenation. The catalytic performance tests illustrated that the selectivity towards total butenes in 1,3-butadiene hydrogenation becomes more than 96% (irrespective of conversion) upon coating the supported nickel catalysts with the IL. Aiming at investigating the structural factors controlling such effect of ILs on supported metal catalysts, single-site supported metal catalysts were prepared and coated with a family of ILs. High energy resolution fluorescence detection X-ray absorption near-edge spectroscopy (HERFD-XANES) and infrared (IR) spectroscopy illustrated a strong correlation between the degree of electron donation from IL coatings to the metal sites and the interionic interaction energy in ILs. The performance testing on these IL-coated catalysts showed that the catalyst becomes more selective for partial hydrogenation with an increase in the degree of electron donation from the IL. These results demonstrate a new class of atomically dispersed supported metal catalyst with tunable electronic environments, opening up new opportunities for precise tuning of the catalytic performance by the choice of IL, which offers an enormous number of different structures with different physical and chemical properties.

Acknowledgment This research is supported by TUBITAK (project number: 113M552).

IL–13

Growth and Shape Stability of Bi-metallic Nano-particles

Sondan Feyiz Durukanoğlu

Kadir Has University, Faculty of Engineering and Neutral Sciences, Department of
Electric–Electronics Engineering, İstanbul – Turkey

Controlling the morphology of non-noble bi-metallic nano-crystals has become the focus of several studies as these nano-stuructures can provide a great opportunity to improve their performance and activity in catalytic reactions. Although much of the focus has been on the overall macroscopic description of synthesis processes, it is still a great challenge to identify the leading factors in a typical crystal growth process at atomic-scale. Here we report results of atomic scale calculations on shape evolution and stability of grown bi-metallic Cu-Ni nano-particles using molecular static and dynamic simulations. Our growth simulations on bare Cu and Ni nano-cubes reveals that single-atom diffusion characteristics play an important role in utilizing the particle with specific morphology and architecture.

IL–14

Long-range Control of Protein Conformations for Function Fine-tuning

Canan Atılgan

Sabancı University, Faculty of Engineering and Natural Sciences, İstanbul – Turkey

While the static three-dimensional protein structure provides an initial understanding of its possible function, it is now well-accepted that the shifts in the dynamics of the protein are exploited to fine tune its performance under slightly varying conditions. However, the physics of how these changes are achieved is not as clear. We have developed computational and theoretical strategies to disclose the mechanisms by which proteins utilize point mutations or shifts in the conditions of the aqueous media to modify functions [1]. Here, we will outline some of those methodologies [2] and discuss examples on how these approaches provide insight to the functioning of proteins with diverse modes of operation such as virus capsids, heat shock proteins and calmodulin [3-6]. To explain the coupling between varying IS/pH in the water environment and conformational changes, we discuss a plausible electromechanical model for proteins [7]. For point mutations, we resort to free energy perturbation calculations coupled with coarse grained identifiers to rationalize entropy/enthalpy compensation. The latter are exemplified by complementary experimental/computational studies of PDZ domains and dihydrofolate reductase [8].

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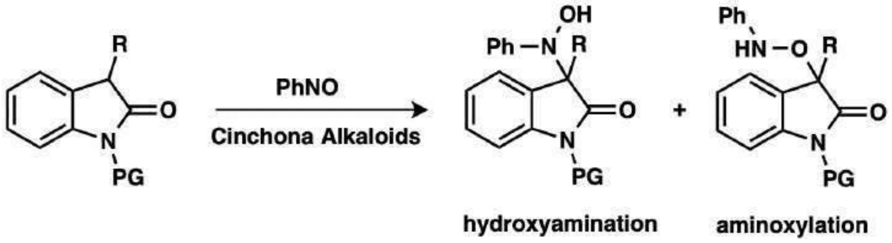
IL–15

Theoretical Active Site Models for Catalyst Discovery

Nihan Çelebi Ölçüm, Sezen Alsancak, Yeşim Çamlısoy

Yeditepe University, Department of Chemical Engineering, İstanbul – Turkey

Determination of efficient and selective organocatalytic structures still is an expensive and challenging method involving the synthesis of a large number of derivatives followed by experimental testing of their catalytic activities. A rational computational organocatalyst design approach1 could accelerate the discovery process.
This lecture will describe how quantum mechanically optimized active site models are coupled with drug design tools to discover a new organocatalyst with no previously known catalytic activity for reactions of oxindoles with nitrosobenzene to address the challenge of catalysis of one of the two competing pathways in a pharmaceutically important target reaction (Scheme1).



Scheme1. Hydroxyamination and Aminoxylation Reactions of 2-oxindoles

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IL–16

Homology Modeling of Mammalian Nav Channels

Ali Osman Acar[1], **Murat Çavuş**[2], **Serdar Kuyucak**[3], **Turgut Baştuğ**[4]

[1]TOBB University of Economics and Technology, MNT Program, Ankara – Turkey
[2]Yozgat Bozok University, Faculty of Education, Yozgat – Turkey
[3]University of Sydney , School of Physics, Sydney – Australia
[4]Hacettepe University, Faculty of Medicine, Department of Biophysics, Ankara – Turkey

Cell membranes consist of two layers of lipid molecules and are impermeable to ions. Ion transportation across the membrane comes true by means of integral proteins such as ion channels. Voltage gated sodium (NaV) channels are essential elements in ion channels family that responsible for the rapid upstroke of the action potential. Any problem that occur in ion channels leads to hereditary epilepsy, migraine, periodic paralysis, cardiac arrhythmia and chronic pain syndromes. Recent crystal structures of Nav channels have made a way to understand their function and mechanism. However, the absence of mammalian structures leads to the progression of these structures through the use of homology modeling techniques. The crystal structures of nine isoforms of sodium channels (Nav1.1- Nav1.9) found in the mammals are unknown. For this reason, structures that have high sequence similarity with mammalian structures are used via homology modeling. In this study, we present a homology model of Nav1.4 mammalian crystal structure obtained by using NavPaS (PDB ID: 5X0M) structure as a template. The validation of the model was made by comparing the tetrodotoxin affinities obtained from computational methods and experiments.

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IL–17

Design and degradation of oligomers and copolymers for organic photovoltaic materials

Viktorya Aviyente

Boğaziçi University, Department of Chemistry, İstanbul – Turkey

In recent years, demand for renewable and sustainable energy sources increased dramatically. Compared to the inorganic materials, organic semiconductors (OSC) have advantages such as easy fabrication, low cost, lightweight and flexibility, but the main drawback of the OSC's is the relatively low efficiency compared to the inorganic material based systems.[1] Convenient band gap between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), extensive absorption spectrum to harvest more sunlight, and well defined crystal structure to improve charge transfer between layers are the important properties that the materials used in OSC's should have. Theoretical calculations are helpful to give us an insight to rationalize or predict the properties of the molecules that are potentially useful in OSC's The study carried on 80 different push-pull type organic chromophores which possess Donor-Acceptor (D-A) and Donor-Thiophene-Donor-Thiophene (D-T-A-T) structures will be discussed. Significant new insights into physical chemistry have been introduced by carrying out methodological benchmark calculations (DFT and TD-DFT) on band gaps, transition dipoles, chain lengths, bond length alternations, distortion energies, reorganization energies, excited-state vertical transitions to predict the optical properties of these systems accurately. Careful analysis of our findings has allowed us to propose potential donor-acceptor couples to be used in organic photovoltaic cells.[2]

On the other hand, π-conjugated polymers played considerable role in the development of the conductive, electrochemically active, light emitting materials after the discovery of electrically conductive polyacetylenes. In this respect, due to their vacant p-orbital, the ability of acting as a π-acceptor while remaining σ-donor and relatively easy corporation with organic molecules, three-coordinate boron compounds have drawn significant attention.[3] Thus the study of excited state topologies, absorption and emission maximums, ϕ_s values, natural transfer orbitals (NTO) and two-photon absorption (TPA) spectra's of a series of bis(E-dimesitylborylethenyl)-substituted arenes and their degradation carried out by means of DFT and TD-DFT will be presented.

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IL–18

Theoretical investigation of new bithiophene-imide (BTI) based organic semiconductors

Berkay Sütay, Erol Yıldırım, Mine Yurtsever

İstanbul Technical University, Department of Chemistry, İstanbul – Turkey

In the past two decades, the organic donor-acceptor type semiconducting copolymers have been extensively investigated for their eligibility in electronic devices. Recently, bithiophene-imide (BTI)[1,2] (Figure 1) based organic molecules were synthesized as new material for organic field effective transistors (OFET). The BTI units as electron acceptor units were linked by the alkyl substituted oligothiophenes as electron donor units. It was reported that the R1 functional group on BTI group and length of the alkyl substituents on thiophene rings effect the self-organization, crystallinity and hence charge transport properties of the copolymers. In this study, the impact of the substituent groups on the optoelectronic and charge mobility properties of different copolymers were investigated thoroughly with density functional theory (DFT) method at the oligomer level. The environmental stability of the copolymers were estimated by studying the adsorption isotherms of water, carbondioxide and oxygen gases with Monte Carlo (MC) method.

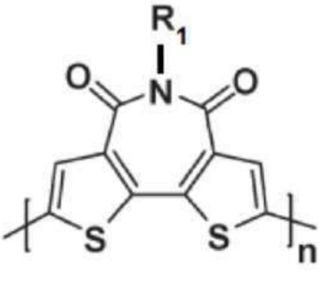

Figure 1: Bitiyofenimid (BTI) monomer unit (R1: H, NO_2, NH_2, OH, F,Cl, Br, I)

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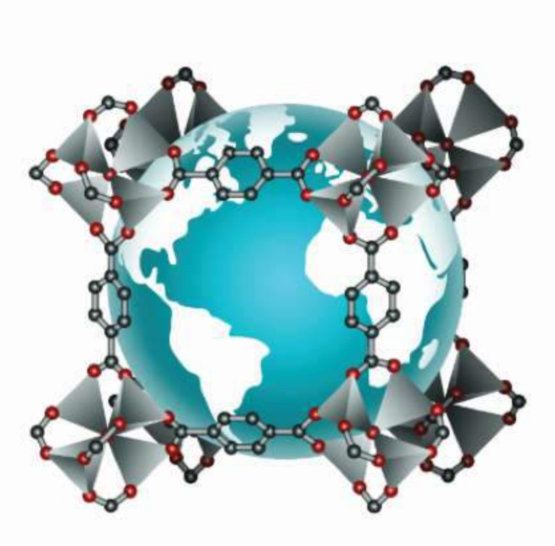
IL–19

Molecular Modeling of Porous Materials: From Energy to Biomedical Applications

Seda Keskin

Koç University, Department of Chemical and Biological Engineering, İstanbul –Turkey

We have witnessed the quick growth of research on a new group of porous materials named as metal organic frameworks (MOFs) in the last decade. MOFs have exceptional physical properties such as low densities, large surface areas and high porosities which make them promising materials for a large variety of applications. MOFs have been recently used for gas storage, gas separation, sensing, catalysis, and drug delivery. The large variety in topologies and chemical functionalities of MOFs offer a large number of materials that can exhibit extraordinary performances compared to traditional porous materials. Considering the large number of existing materials, it is not practically possible to test every single MOF material for a target application using purely experimental manners. Our research group uses molecular simulation techniques to perform large-scale screening of MOFs with the aim of identifying the best performing materials for desired applications. In my talk, I will show our recent results on using molecular modeling methods to unlock the potentials of MOFs for gas storage, gas separation, drug storage and drug delivery. I will also discuss structure-property relationships for MOFs which can serve as a map for the design and development of new MOFs with better performances.



CPC–XII: 12th Chemical Physics Congress

ORAL PRESENTATIONS

OP–1

Atomistic and mesoscopic simulations to study structure and properties of PEG and water mixtures

Gökhan Kaçar

Trakya University, Department of Genetics and Bioengineering, Edirne – Turkey

In this work, we employ molecular simulations at different scales in order to study the mixing properties, structure and material properties of polyethylene glycol (PEG) and water mixtures. PEG is a widely studied material, and a thorough understanding of its molecular structure and properties in bulk and in water is significant to predict its behavior in more complicated environments. Therefore, we Initially perform Dissipative Particle Dynamics (DPD) simulations [1] to mimic the experimental negative volume excess of PEG and water mixtures [2]. The hydrogen bond attraction, which is the main energetic contribution to the volume shrinkage, is incorporated in DPD by modifying its non-bonded potential [3]. To that purpose, a Morse potential term is added to the conservative repulsive DPD potential. DPD simulations predict not only the phase behavior of PEG-water mixtures, but lead to the proper representation of the PEG chain configurations in dry and wet environments. A significant degree of chain helicity is observed from DPD simulations, where the helical structures are favored in water compared to dry environment in line with the experiments [4]. Following the creation of mesoscopic PEG structure in water, we run atomistic molecular dynamics simulations to monitor the chain configuration and material properties of PEG in dry and wet conditions. Bridging mesoscopic and atomistic length scales is done by a reverse-mapping procedure [5], where atomistic detail is inserted into mesoscopic coordinates. As a result, material properties such as coefficient of thermal expansion, elastic modulus and Poisson's ratio are computed [5]. It is observed that the computed values reveal that PEG becomes more elastic and less compressible upon addition of water.

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OP–2

Mechanism of the GTP Hydrolysis in Elongation Factor EF-Tu

Bülent Balta[1], Gülşah Çifci[2], Şeref Gül[3], Mehtap Işık[4], Selami Ercan[5],
Ayla Başaran Kınalı[1], Berke Türkaydın[1], Viktorya Aviyente[2], Neş'e Bilgin[6]

[1]İstanbul Technical University, Department of Molecular Biology and Genetics, İstanbul – Turkey
[2]Boğaziçi University, Department of Chemistry, İstanbul – Turkey
[3]Koç University, Department of Chemical and Biological Engineering, İstanbul – Turkey
[4]Weill Cornell Graduate School of Medical Sciences, Tri-Institutional PhD Program in Chemical Biology, New York – United States
[5]Batman University, School of Health, Batman – Turkey
[6]Boğaziçi University, Department of Molecular Biology and Genetics, Istanbul – Turkey

Elongation Factor Tu (EF-Tu), when bound to GTP, forms a complex with amino acyl-tRNA and delivers it to the ribosome. Cognate codon-anticodon pairing causes conformational rearrangements on the ribosome, aa-tRNA and EF-Tu. As a result, GTP is hydrolyzed, EF-Tu leaves the aa-tRNA in the ribosome and moves away [1]. Although EF-Tu also has an intrinsic GTPase activity, the ribosome stimulated hydrolysis is 10^6-fold faster. It is known that a conserved histidine and the P-loop are important for catalysis [2]. However, their exact roles are controversial. Although in other G-proteins, an arginine is also involved, a corresponding residue is not identified on EF-Tu.

In this study, using molecular dynamics simulations on the wild type and mutant EF-Tu from *E. coli* and *T. aquaticus*, we show that the catalytic histidine and P-loop are not sufficient to account for the high stimulatory effect of the ribosome. In the *T. aquaticus* simulations, the Switch I region, an α-helix near the active site, explores several conformations and R57 of Switch I enters the active site like the catalytic arginine in other G-proteins. Potential of mean force calculations show that this process can occur through a low activation barrier in the binary EF-Tu·GTP complex. However, in the ternary EF-Tu·GTP·tRNA complex, the mobility of Switch I is reduced. QM/MM calculations indicate that only when both the catalytic histidine and arginine are situated in the active site, an activation energy consistent with experiments can be obtained.

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OP–3

Electronic Structure of BOPHY – When Does Adding Two Rings Not Make a Larger Ring?

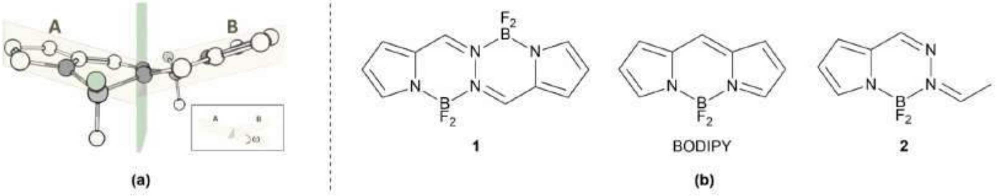
Muhammed Büyüktemiz, **Yavuz Dede**

Gazi University, Faculty of Science, Department of Chemistry, Ankara – Turkey

Florescent organic molecules are central to a great number of fundamental and applied chemical systems. Fine tuning the fluorescent properties of organic fluorophores is generally accomplished via modifications on the π–framework. An alternative approach of high potential, lies in the design of the new π–cores.

Recently, Ziegler et. al. reported[1] the synthesis of a new fluorescent dye, BOPHY(1), with a high fluorescent quantum yield. **1** is structurally very similar to BODIPY[2], a very well-known fluorophore however, photophysical properties of **1** are surprising. Despite being a larger π–system, BOPHY absorbs at a lower wavelength than BODIPY and is predicted to be non-planar in quantum chemical calculations yet XRD studies suggested a planar structure.

Herein, we report a detailed quantum chemical analysis (MCSCF, DFT, MD-DFT, TD-DFT, MP2) of **BOPHY** in comparison to **BODIPY** and **2** (Figure 1b). Structural, electronic and energetic properties of **1** led us to conclude that it has a non-planar minimum energy geometry in both ground and excited states and the planar geometry corresponds to a transition state structure. Planarity in XRD is shown to be induced by π–interactions inherent in the crystal structure. Furthermore, **1** is shown to be composed of electronically isolated monomers of **2** and is not aromatic, hence the unexpected blue shift with respect to BODIPY. Our calculations predicted new spectroscopic features for **1** and were confirmed successfully.



(a) Puckered structure of BOPHY, interplanar angle between A and B is 28°. (b) Molecules studied in this work.

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OP–4

Developing Force Fields For Novel Drug Candidates Using QM

Emre Gürsoy[1], **Turgut Baştuğ**[2]

[1]TOBB University of Economics and Technology, Ankara – Turkey
[2]Hacettepe University, Faculty of Medicine, Department of Biophysics, Ankara – Turkey

Due to high cost of the drug development process and the rapid development in computer technology, computer aided drug design has become popular in drug development. Molecular modeling plays a major role in the computer aided drug design process. Current Force Fields (CHARMM, AMBER, GROMACS, etc.) do not have the parameters of drug candidates, so it is not possible for newly developed drug candidates to perform computer based Molecular Dynamics simulation.
Force field parametrization is achieved by doing MP2 / 6-31G* for geometry optimization, calculating Single Point energies for water molecules using HF / 6-31G* and using those energies to find charge properties. MP2 / 6-31G* Hessian calculations are performed for Bond and Angle terms and finally MP2 / 6-31G* level QM calculations have been done in order to get dihedral terms.
The main objective of this work is to develop CHARM compatible Force Field parameters for the novel GST P1 inhibitor ($C_{19}H_{13}N_5O_5$). The validation of the generated Force Field is achieved by Molecular Dynamics simulation.

OP–5

Testing the limits of Applicability of the Perturbation Response Scanning Method via Small Molecule Toy Models

Kurt Arıcanlı, Canan Atılgan

Sabancı University, Faculty of Engineering and Natural Sciences, İstanbul –Turkey

As the Levinthal Paradox famously states, the total possible conformations of a typical protein molecule is gargantuan (10^{30}), and the effects of changes in a protein's environment render the timescale of a change in protein secondary and tertiary structures on orders as slow as seconds. Experimentally, protein dynamics on the millisecond scale can be studied using single molecule force spectroscopy [1] or ultraviolet-circular dichroism. [2] On the sub-nanosecond scale, time-resolved protein characterization by infrared spectroscopic [3] methods *in vitro* have limits in residue number (typically > 200 amino acids) and analytical strength. Computerized Molecular Dynamics (MD) reliably simulates the molecular behavior of proteins in a plethora of environments on a microsecond scale *in silico*.

Perturbation Response Scanning [4] (PRS) is a computational method used for obtaining, for a given change in conformation, the hot residues and force vectors. [5] However, the extent to which PRS may be used to aid in sampling protein conformational surfaces is limited due to the limited sampling available for such large molecules. In our study, we have utilized small molecules whose conformational space may be accessed completely by MD within reasonable computation time. It is then possible to apply the PRS method to judge its applicability to switch between any pair of known conformations. We showed, for transitions with identical free energy barriers - *degenerate* transitions - that the PRS outputs - hot residues, force vectors, and propensities - of the transition are identical. Building on this realization, the objective of further work aims to find an analogous relationship between any of the PRS outputs and free energy barriers for non-degenerate transitions for simple molecules whose conformational spaces are readily obtainable using MD.

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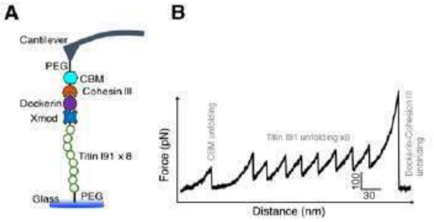
OP–6

Effect of Cantilever Response Time and Hydrodynamic Forces on Force Spectroscopy Measurements

Fidan Sümbül, Felix Rico

Aix-Marseille Université, Institut de Neurosciences des Systéms, Marseille – France

The folding of proteins into their native conformations to perform function is one of the most essential processes within the living cell. Force spectroscopy (FS) using nanotools, such as magnetic tweezers, optical tweezers and AFM, allows the manipulation of individual proteins and monitoring of the forces required to unfold individual protein domains or subdomain. This method provides information about the mechanisms of folding and unfolding under an applied force, allowing the characterization of the (un)folding energy landscape along the axis of applied force. Dynamic force spectroscopy (DFS) is a powerful single-molecule approach that a probe functionalized with a biomolecule is moved at a range of velocities and the resulting unfolding or unbinding forces are recorded [1,2]. Recent theoretical developments suggested a contribution of the finite response time of the probe to the measured forces [3]. To assess this effect, we determined the unfolding forces of individual titin I91 domains using high-speed force spectroscopy4 with cantilevers with a range of response times (milli- to microsecond). In agreement with predictions, our results suggest a non-negligible effect when the unfolding time approaches the response time of the cantilever. This effect overestimates the unfolding forces of titin I91 by 10% at the highest speeds accessible to each cantilever. This contribution might be considered as small for titin I91 unfolding but might be more important for other processes like receptor-ligand unbinding, where rupture forces tend to me smaller.



Experimental design. (A) Schematic representation of the experimental setup showing the site-specific pulling configuration. (B) A force-distance trace showing complete unfolding of the construct

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OP–7

Modeling Photophysical Processes in Push-pull Organic Dyes: Implications for Light Harvesting and Charge Transfer

Esma B. Boydaş[1], **Özlem Şengül**[2], **Mariachiara Pastore**[3], **Philip C. Gros**[4], **Antonio Monari**[3], **Şaron Çatak**[2]

[1]Ruhr-Universitat Bochum, Lehrstuhl für Theoretische Chemie, Bochum – Germany
[2]Boğaziçi University, Department of Chemistry, İstanbul – Turkey
[3]Université de Lorraine, Théorie-Modélisation-Simulation, Nancy – France
[4]CNRS, Hecrin SRSMC, Nancy – France

To provide a low-cost alternative to silicon and other inorganic-based photovoltaic devices, employing fully organic dyes as sensitizers has recently gained considerable attention, following Gratzel's invention of Dye-Sensitized Solar Cells (DSSCs). [1] A novel class of organic dyes, emerging as promising donor substitutuents in D-π-A sensitizers were appraised in terms of linear and nonlinear optical properties. A conformational analysis was performed on 2,5-dithienylpyrrole (DTP) [2] dyes. Absorption spectra was obtained at Time Dependent Density Functional Theory (TD-DFT) while including dynamical effects via a Wigner distribution 3 in the ground vibrational state. Excited state topologies and charge transfer character of the dyes were quantified with recently developed methodologies: calculations of ϕ_s index [3,4] and Natural Transition Orbitals (NTOs) [5]. Two-photon absorption (TPA) [6] abilities were also reported, which show significantly high cross-sections in the IR region, thus making the two organic dyes good candidates for non–linear optical applications. In addition to the work in isolated dyes, density functional theory (DFT) calculations have been performed to elucidate the dye-semiconductor electronic injection process – the first step of charge generation in solar cells. Projected density of states (PDOS) showed a lack of intrinsic charge transfer nature in the dyes.

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OP–8

Proposing Novel MAO-B Hit Inhibitors Using Multidimensional Molecular Modeling Approaches

Yusuf Serhat İş[1,2,4], **Serdar Durdağı**[1,3], **Busecan Aksoydan**[1,3], **Mine Yurtsever**[2]

[1]Bahçesehir University, School of Medicine, Department of Biophysics, Computational Biology & Molecular Simulations Laboratory, İstanbul – Turkey
[2]İstanbul Technical University, Department of Chemistry, İstanbul – Turkey
[3]Bahçesehir University, Graduate School of Health Sciences, Neuroscience Program, İstanbul – Turkey
[4]Bahçesehir University, Vocational High School, Department of Chemical Technology, İstanbul Gedik University, İstanbul – Turkey

Monoamine oxidase (MAO) enzymes MAO-A and MAO-B play a critical role in the metabolism of monoamine neurotransmitters. [1] The function of MAOs is to catalyze the oxidative deamination of monoamine neurotransmitters like dopamine, serotonin and norepinephrine. [2] Hence, MAO inhibitors are very important for the treatment of several neurodegenerative diseases such as Parkinson's disease (PD), Alzheimer's disease (AD), and amyotrophic lateral sclerosis (ALS). In this study, 256750 molecules from Otava Green Chemical Collection were virtually screened for their binding affinities to MAO-B enzyme. Two hit molecules were identified after applying different filters such as high docking scores and selectivity to MAO-B, desired pharmacokinetic profile predictions with binary quantitative structure–activity relationship (QSAR) models. Therapeutic activity predictions, pharmacokinetic and toxicity profiles were investigated using MetaCore/MetaDrug suite. However molecular dynamics (MD) simulations were performed to make more detailed elucidations beyond docking and pharmacokinetic prediction studies. All these calculations were made also to find out whether the two candidate molecules carry MAO-B selectivity versus MAO-A. We identified one hit molecule (ligand 1, Otava ID: 3463218) which displayed higher affinity and selectivity toward MAO-B than a positive control compound selegiline which is a commercially used in the treatment of Parkinson's disease.

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OP–9

Comparison of thermal, crystal and magnetic properties of NiTi and NiTi-Co shape memory alloys

Mediha Kök, Hanaa Shahab Ahmead Zardawi

Fırat University, Department of Physics, Elazığ – Turkey

Equal atoms NiTi shape memory alloys have many areas from biomedical to automobile industry. For this reason, there is considerable demand for such shape memory alloys. The increase in the demand for NiTi based alloys motivates the researches to investigate these alloys extensively. This study examined the positive or negative aspects of cobalt element on different atomic percentages of NiTi alloy. NiTiCo shape memory alloys were produced by arc melter method and melting process was done for several times to ensure homogenized. Differential Scanning Calorimetry (DSC) for thermal analysis, x-ray device for crystal structure analysis (XRD) and PPMS device for magnetic measurements were used to investigate effects of cobalt element. According to experimental results, the transformation temperatures increased by the increase of the nickel, cobalt and titanium ratios in the NiTiCo alloy. The crystal structure of the B2 martensite phase, the Ti_2Ni phase and the Rombohedral phase Ni_4Ti_3 phase were determined by XRD measurement.

Acknowledgment This work has been supported by the Management Unit of the Scientific Research Projects of Firat University (FUBAP) (Project Number: FF.18.11).

OP–10

Electronic Structure-FunctIon Relationship in Solar Cells and Bio-Inspired Fe Catalysts

Özlen F. Erdem

METU, GÜNAM, Ankara – Turkey

Materials which are used for photovoltaic energy conversion, in particular thin-film silicon solar cells and perovskites, can have drastically improved solar conversion efficiency when their impurities, defect centers, and light-induced structural changes are controlled. Knowledge about the genesis and electronic structure of defect states at an atomic level is essential, even prerequisite, for optimizing the efficiency of the solar cells. Defect states in silicon are often paramagnetic or can be made paramagnetic through electrically, optically, or structurally induced processes, e.g. charge separation or photo-induced charge transfer. Nanoscopic insight into their structural and functional properties can be obtained by magnetic interaction of the magnetic moments with each other and/or the host matrix. In this presentation, after a brief introduction of spin dynamics, electronic structure of such energy materials will be discussed with an emphasis on the spin properties of the relevant electrons. In addition, investigation of the electronic structure-function relationship of bi-inspired Fe catalysts will be presented.

OP–11

Mechanism of CO_2 and H_2 Adsorption on Different Cu211 Surfaces: a Density Functional Theory Study

Derya Düzenli[1], **lker Tezsevin**[2,3], **Işık Önal**[3]

[1]Mineral Analysis and Technology, General Directorate of Mineral Research and Exploration, Ankara – Turkey
[2]Dutch Institute for Fundamental Energy Research, Eindhoven – The Netherlands
[3]METU, Chemical Engineering Department, Ankara – Turkey

The first two stages of the catalytic conversion of CO_2 into methanol over Cu211 and metal-doped Cu(211) surface has been studied by means of density functional theory (DFT) calculations. The interactions of CO_2 and H_2 on bare and doped Cu(211) surfaces at various adsorption sites are investigated for different gas molecule orientations to determine the most stable adsorption sites and geometries as a first step of the study. The metal-doped surfaces are prepared by adhesion of various amounts of gallium (Ga) and holmium (Ho) atoms on the (211) surface of Cu catalyst. Our results show that adsorption of reactants over Ho-doped Cu(211) surface is thermodynamically more favorable than the other surfaces. Additionally, the reactants adsorption energies increase with the increasing of Ho atom numbers. In the second step, the reactions between adsorbed species resulting in the formation of formate (COOH) and carboxyl (HOCO) intermediates are investigated. The calculation results show that hydrogenation of CO_2 occurs via different pathways on Ho and Ga doped Cu(211) surfaces. HOCO forms over Ho-doped Cu(211) surface while HCOO forms over bare and Ga-doped Cu(211) surfaces.

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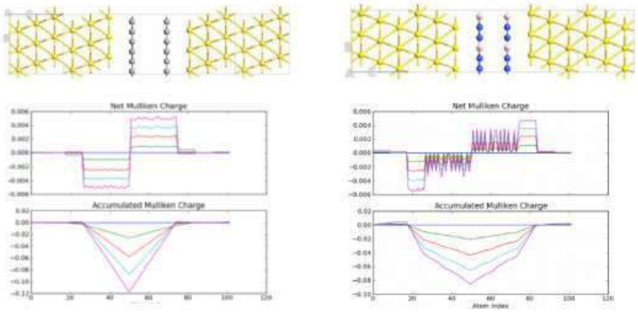
OP–12

Investigation of Energy Storage Capabilities of Graphene and h-BN Double Layer Electrostatic Supercapacitor

Nazan Kara[1,2], **Hatice Kökten**[1], **Cem Özdoğan**[3]

[1]METU, Department of Physics, Ankara – Turkey
[2]Çankaya University, Graduate School of Natural and Applied Sciences, Ankara – Turkey
[3]İzmir Katip Çelebi University, Department of Engineering Sciences, İzmir – Turkey

In this study, graphene and hexagonal boron nitride (h-BN) sheets were investigated theoretically as 2-dimesional planar electrodes in nano size capacitors. Quantum capacitance and energy storage capacities of perfect (pristine) model systems formed in different geometries and shapes will be reported. Quantum mechanical calculations were performed using the Density Functional Theory (DFT) based Non-equilibrium Green's Function (NEGF) method. By providing convergence, the quantum transport quantities as well as the charge distributions and the capacitance of the system can be found. Calculation of the capacitance properties of the electrode-device-electrode systems was carried out using ATK (Atomistix ToolKit) package program. The non-polarized GGA / PBE + NEGF approach was used in the calculations. The wave functions are expressed by the basic sets of DZP (Double-Zeta-Polarized), which are local numerical atomic trajectories. Structural optimization of the working systems was done by the Fast Inertial Relaxation Engine (FIRE) method. The preliminary results obtained by Mulliken analysis are 2.18x10^{-20} F (0.18x10^{-20} F) for quantum capacitance, 3.37 μF/cm^2 (2.26 μF/cm^2) for spesific capacitance and 29.64 F/g (45.61 F/g) for gravimetric capacitance of graphene (h-BN) model capacitor system.



Acknowledgments This work is supported by The Scientific and Technological Research Council of Turkey (TUBITAK) through the project No: 115F137. Our numerical calculations were performed at TUBITAK ULAKBIM, HighPerformance and Grid Computing Center (TRUBA resources).

OP–13

Synthesis of Poly(Azomethine)s Derived From Dialdehyde and Phenazopyridine Hydrochloride: Characterization, Thermal and Spectroscopic Studies

Feyza Kolcu

Çanakkale Onsekiz Mart University, Lapseki Vocational School, Department of Chemistry and Chemical Technologies, Çanakkale – Turkey

An alternate method to synthesize conjugated polymer is the use of azomethine (–N=C–) connections. Conjugated poly(azomethines), polyimines, or poly(Schiff bases) are another interesting class of conjugated polymers containing nitrogen atoms in a polymer backbone.[1] Among the rich chemistry of various semiconductors, the conjugated compounds with CH=N Schiff base linker, seem to be attractive for optoelectronics. The main representatives of this family are azomethines, also named Schiff bases or imines. [2,3] Poly(azomethine)s possess the ability to form liquid crystals and complexes with metals, are characterized in terms of high thermal stability and exhibit therapeutic activity, therefore they are widely used in different fields such as analytical chemistry, organic synthesis, medicine, biology, as well as in organic electronics as electrochromic material and photovoltaic (OPV) cell components. [4]

In this study, two poly(azomethine)s were prepared via polycondensation chemistry in which two formerly synthesized dialdehydes were reacted with phenazopyridine hydrochloride to give a Schiff base polymer in a simple one-step process of polycondensation.

The chemical structure of the synthesized compounds was characterized by the FT-IR, UV-Vis, ^{1}H-NMR and ^{13}C-NMR techniques. Further characterization was employed using thermogravimetric analysis-differential thermal analysis (TG-DTA), fluorescence (PL), electrochemical-cyclic voltammetry (CV) and differential scanning calorimetry (DSC) measurements. The number of average molecular weights of polymers was calculated using GPC instrument. Scanning Electron Microscopy (SEM) images were illustrated to explore the morphologic property.

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OP–14

Ab-initio Applications Thermodynamics in Surface Science and Heterogeneous Catalysis

M. Oluş Özbek

Yeditepe University, Chemical Engineering Department, İstanbul – Turkey

Density Functional Theory (DFT) has been used in chemistry for the last three decades and has proven itself to be reliable and strong tool. Furthermore, introduction of the periodic techniques enabled scientists to better represent and understand the infinitely large surfaces, an area which the cluster models lacked.

When applied for a system, DFT solves for the electronic structure at zero temperature and zero pressure conditions. The basic results such as electronic energy, electronic structure and geometry are sufficient for most of the cases. Even under these conditions DFT stands as an irreplaceable tool to study the unobservable phenomena such as transition states and metastable structures. However, at an initial glance relating these basic DFT results to real life applications may appear confusing or unrealistic. At this point it is crucial to understand that these basic results contain the relevant information needed to describe the effect of temperature on the atomic level. Through the combination of the DFT results and thermodynamic relations it is possible to reach finite temperature and pressure conditions. Furthermore, this methodology enables the study of the larger systems by dividing them into smaller subsystems, whose interactions are governed by thermodynamic laws. This kind of application is especially useful for the study of surface reactions, where a solid surface (solid phase) is interacting with a gas phase. This makes DFT yet another efficient tool to study and understand the catalytic systems by filling the physically unobservable gaps.

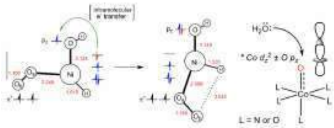
OP–15

Two Short Stories on Radical Centers Involved in Non-radical Reactions: Dioxygen Activation by $[(\mathrm{H})\mathrm{Ni}(\mathrm{OH})]^+$ and Water Oxidation at Co-Oxo/Oxyl

Yavuz Dede

Gazi University, Department of Chemistry, Faculty of Science, Ankara – Turkey

Radical intermediates featuring unpaired electrons play key roles in chemical reactions. Transition metal centers performing bond activation and/or catalysis are not-surprisingly found in electronic states where there are a ‘good’ number of unpaired electrons occupying - commonly metal based - frontier molecular orbitals involved in electron transfer, change of spin state, and related phenomena pertaining to reactivity. Thus, the significance of a reactive radical intermediate in a reaction mechanism is generally sought in electrons pairing and unpairing. In questioning this general view on radicals, two thought-provoking examples will be communicated. First, high level ab initio calculations on $[(\mathrm{H})\mathrm{Ni}(\mathrm{OH})]^+$ complex cation,[1,2] that activates dioxygen as well as methane in separate reactions, suggests that the reactive first excited quartet state bearing radical centers on both oxygen and Ni atoms, is activating the triplet radical dioxygen in a thermal way. The two radical centers were not involved in radical coupling with the substrate. Secondly various penta-coordinated Co(III/IV) centers catalyzing water oxidation via attack of water to Co(III/IV)–O are repeatedly shown to follow the nucelophilic mechanism.[3,4] High level ab initio calculations suggest that the Co–O center is in an overall quartet spin electronic configuration featuring the $|\mathrm{Co(d)}(\uparrow)\rangle$ $|\mathrm{Co(d)}\pm\mathrm{O(p)}(\uparrow)\rangle$ $|\mathrm{Co(d)}\pm\mathrm{O(p)}(\uparrow)\rangle$ occupation motif. The distribution of spin along the Co–O bond seems to be the key for the quartet center avoiding radical reaction.



Activation of triplet dioxygen by quartet $[(\mathrm{H})\mathrm{Ni}(\mathrm{OH})]^+$(left). O–O bond formation at the quartet Co(IV/III)–oxo/oxyl center (right).

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CPC–XII: 12th Chemical Physics Congress

POSTER PRESENTATIONS

PP–1

Catalyst Discovery for the Reaction of Oxindole With Nitrosobenzene With a New Computational Method

Yeşim Çamlısoy, Sezen Alsancak, Nihan Çelebi Ölçüm

Yeditepe University, Department of Chemical Engineering, Istanbul – Turkey

The number of reports on the use of small chiral organic molecules as catalysts and related computational efforts for understanding the origins of catalysis and selectivities keep growing at a breathtaking pace. Quantum mechanical calculations have successfully uncovered numerous organocatalytic reaction mechanisms and explained the observed reaction outcomes. Yet, the prediction of effective catalysts is still a challenging task. The determination of effective and selective organocatalytic structures still largely relies on serendipity, and experimental trial and error. The purpose of this project is to allow easy and cost-effective determination of potential organocatalyst candidates for a target reaction using a new computational approach that combines the quantitative power of quantum mechanical calculations with drug design tools. The proposed method aims to decrease the cost of experimental screening by allowing the determination of organocatalysts with the desired three-dimensional arrangement of catalytic functional groups in an organocatalyst pool. Because the oxindole skeleton bearing a tetrasubstituted carbon at the 3-position is a special motif forming the core of many bioactive natural products and pharmaceutically active compounds[1], the development of chiral catalysts for their asymmetric synthesis is among the most actively studied topics in recent years. For this reason, for the application of the proposed approach in this project, the reactions of oxindoles with nitrosobenzene were selected as targets. In the presence of amine catalysts, it gives two different products (hydroxyamination and aminoxylation products) and both of these products display different bioactivities and therefore, their selective synthesis is very important in pharmaceutical industry. In this work[2], effective and selective organocatalysts for the reaction of oxindole with nitrosobenzene were explored at the B3LYP/6-31G(d) level of density functional theory (DFT).

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PP–2

Electronic origin of the AlH_4 dissociation on various metal (111) surfaces: A DFT study

Ali Emre Genç[1], **Aykan Akça**[2], **Bülent Kutlu**[1]

[1]Gazi University, Faculty of Science, Department of Physics, Ankara – Turkey
[2]Aksaray University, Faculty of Science, Department of Physics, Aksaray – Turkey

As very well known, the mankind need to substitute fossil fuels with more benign sources for the environment and excess resources for the usage in order to prevent complicated effects of the global warming. At this point, hydrogen is one of the most promising resources among the other renewable sources such as wind, solar and nuclear energies [1]. Metal aluminum hydrides ($MAlH_4$, M=Li, Na etc.) are very important for their high gravimetric hydrogen content. Catalytic effect should be considered to remove hydrogens from these compounds. Metal aluminum hydrides are composed of alkali metal atom (M^+) and molecular aluminum hydride (${AlH_4}^-$) unit. The hydrogen atoms are covalently bonded to the Al atom. ${AlH_4}^-$ is a borohydride-like molecule and can be investigated on metal surfaces because they form overall neutral cell together [2,3].
In this work, sequential decomposition mechanism of the neutral AlH_4 molecule on Al(111), Ag(111), Au(111) and Cu(111) surfaces have been investigated. Initially, most stable geometries of AlH_x (x=1→4) species were found. Then, hydrogen atom and AlH_x (x=3→0) species were co-adsorbed and transition state energies and geometries were found. Density of states (DOS), Mulliken charge analysis and electron density differences (EDD) were used to discuss the electronic origin of the activity differences between surfaces. According to our results, initial AlH4 dehydrogenation reactions run against to each other on all surfaces. Cu(111) and Au(111) surfaces compete with each other along the reaction pathway. However, overall activation barrier of Cu(111) surface is less than the others for aluminium hydride decomposition reaction on various metal surfaces. Transition state geometries and energies were calculated through LST/QST method [4] within Material Studio CASTEP simulation package [5].

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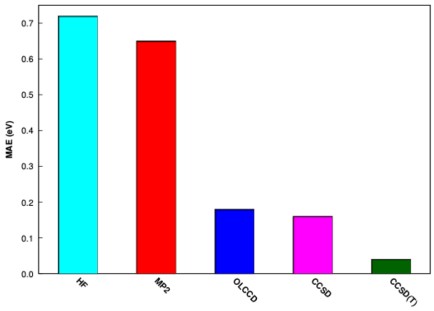
PP–3

State-of-the-art Computations of Vertical Ionization Potentials With the Extended Koopmans' Theorem Integrated With the CCSD(T) Method

Uğur Bozkaya, Aslı Ünal

Hacettepe University, Department of Chemistry, Ankara – Turkey

The accurate computation of ionization potentials (IPs), within 0.10 eV, is one of the most challenging problems in modern computational chemistry. The extended Koopmans' theorem (EKT) provides a systematic direct approach to compute IPs from any level of theory. In this study, the EKT approach is integrated with the coupled- cluster singles and doubles with perturbative triples [CCSD(T)] method for the first time. For efficiency, the density-fitting (DF) approximation is employed for electron repulsion integrals. Further, the EKT-CCSD(T) method is applied to a set of 23 molecules, denoted as IP23, for comparison with the experimental ionization potentials. For the IP23 set, the EKT-CCSD(T) method, along with the aug-cc-pV5Z basis set, provides a mean absolute error of 0.05 eV. Hence, our results demonstrate that direct computations of IPs at high-accuracy levels can be achieved with the EKT-CCSD(T) method. We believe that the present study may open new avenues in IP computations.



Acknowledgment This research was supported by the Scientific and Technological Research Council of Turkey (TÜBİTAK)-114Z786).

PP–4

On the Potential Use of Polyfluorinated Dendrimeric Phthalocyanines as Photosensitizers in Photodynamic Therapy: a TD–DFT Survey

Başak Koca[1], **Şaron Çatak**[1], **Antonio Monari**[2], **Viktorya Aviyente**[1]

[1]Boğaziçi University, Department of Chemistry, İstanbul – Turkey
[2]Université de Lorraine and CNRS, LPCT, Nancy – France

Over the past two decades, phthalocyanine compounds have been extensively used as photosensitizers for photodynamic therapy of cancer [1]. Photodynamic therapy is a promising tumor treatment in which visible light is used in conjunction with a non-toxic photosensitizer in an oxygen-rich environment [2]. To destroy the living cells, singlet oxygen must be activated by energy transfer mechanism from the photosensitizing compound; phthalocyanines are good candidates for this treatment due to their strong absorption in the red region of the visible spectrum and high singlet oxygen quantum yield [3].

Besides, there may be predominant reasons which may improve the photosensitizer's singlet oxygen generation efficiency such as solvent effect, electron donating character of substituents and interactions between macrocyclic rings [4] . These parameters influence the triplet state energy, and hence intersystem crossing probability, and ultimately determine phthalocyanine propensity to activate the singlet oxygen. Additionally, they may cause the shift of the Q-Band in electronic spectra.

Time-dependent density functional (TD-DFT) approaches allow the extension of the accurate ground state DFT efficiency to excited states [5]. We have thus undertaken the computational task of investigating the optical properties of pentafluorobenzoxy-substituted phthalocyanines [6] as well as of their unsubstituted analogues to foresee whether they might be used as photosensitizers in photodynamic therapy.

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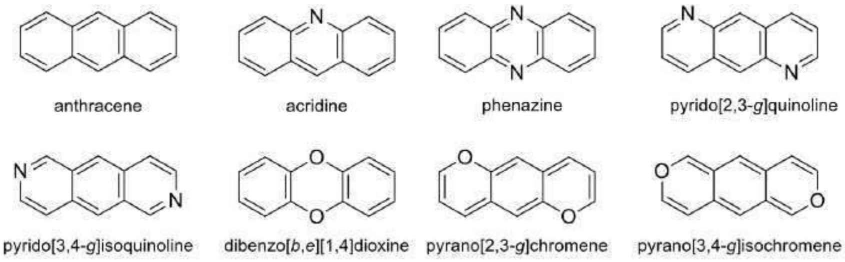
PP–5

Quantum Chemical Analysis of Intersystem Crossing in Organic Fluorophores

Dilara Berna Yıldız, Muhammed Büyüktemiz, Yavuz Dede

Gazi University, Faculty of Science, Department of Chemistry, Ankara – Turkey

Intersystem crossing, a spin-orbit-coupling-dependent internal conversion, mostly takes place from the lowest excited singlet state (S1) to the lowest triplet state (T1) of the molecule in a radiation-less fashion.[1] Excited states of molecules in Figure 1 were studied with MSCSF technique. Relative energies and details of the wave functions were examined for all low lying states. Similarities in excited state wave functions to the previously reported [2] doubly-substituted-tetra-radical (DS-TR) character were particularly studied as a rough measure of ISC probability.



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PP–6

Study on Photophysical Properties of -phenyl-5-(Pyridin-4-yl)-4h-1,2,4-triazole-3-thiol

Cahit Örek[1], **Niyazi Bulut**[2]

[1]Fırat University, Faculty of Science, Department of Physics, Elazığ – Turkey
[2]Kastamonu University, Research and Application Center, Kastamonu – Turkey

Photophysical properties of organic compounds will give insight into their electronic states, from which a lot of information can be obtained to design a new molecule and perform in specific applications. These properties include quantum yield, fluorescence decay time, absorption and fluorescence spectral shift [1]. The 1,2,4-triazole moiety is an important system that is present in a large number of compounds with a wide variety of uses in many fields, such as medicinal chemistry, materials science, and organocatalysis. However, despite the growing number of publications describing the biological and technical applications of triazoles, there are still insufficient data on the photophysical properties of this group.

In this work, photophysical properties of 4-phenyl-5-(pyridin-4-yl)-4h-1,2,4-triazole-3-thiol has been investigated in three solvents of different polarities and absorbance and fluorescence spectra of the title compound was recorded. The obtained experimental results were compared with the 4-phenyl-5-(pyridin-4-yl)-4h-1,2,4-triazole-3-thiol results obtained at B3LYP/6-311++G(d,p) [2] level of theory.

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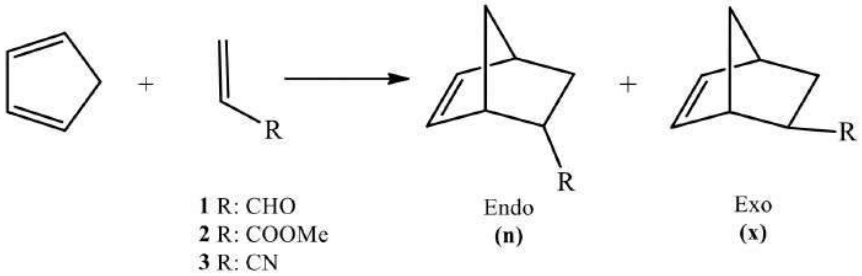
PP–7

Role of Ionic Liquids on the Selectivity and the Rate of Organic Reactions: A Computational Approach

Deniz Akgül, Sesil Agopcan–Çınar, Viktorya Aviyente

Boğaziçi University, Department of Chemistry, İstanbul – Turkey

The Diels-Alder reaction is one of the most common carbon-carbon bond forming reactions used to prepare cyclic compounds in organic chemistry.[1] One of the most interesting aspects of this reaction is its known solvent dependency which enhances reactivity and selectivity.[2] Therefore, choosing an appropriate solvent for this organic reaction is an important task. Although water is a good solvent due to its nontoxicity and increasing rate of reaction, most organic adducts are not soluble in water, so water has been replaced step by step with ionic liquids.[3] The Diels-Alder (DA) reactions between cyclopentadiene (**CP**), acrolein (**1**), methyl acrylate (**2**) and acrylonitrile (**3**) in ionic liquids such as ([Emim][N(Tf)$_2$]), ([Hbim][N(Tf)$_2$]) and ([Bmim][OTf]) have been modeled with density functional theory to explore the effect of ionic liquids on the endo selectivity in the adducts (Scheme 1).



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PP–8

Computational Study On Potential Inhibitors For Protein Kinase CK2 Enzyme

Doğa Özşen, Hande Abeş, Sezen Alsancak, Yeşim Çamlısoy, Nihan Çelebi Ölçüm

Yeditepe University, Department of Chemical Engineering, Istanbul – Turkey

The serine/threonine protein kinase, CK2 (casein kinase 2) can be found in many cells in human body and it is classified as a messenger-independent protein. CK2 has shown a significant role in increasing cell growth for both normal and cancer cell, in addition it acts as a suppressor of apoptosis thus it has been associated with cancer. [1–3] In order to decrease the activity of CK2, development of new inhibitors is a widely studied topic in recent years. CX-4945, also known as Silmitasertib, (5-(3 chlorophenylamino)benzo[c][2,6]naphthyridine-8-carboxylic acid), is the only potential inhibitor for CK2 that has been passed to phase 2 in clinical trials as a drug. CX-4945 is an orally administered, highly specific, ATP-competitive inhibitor of CK2 and it shows cytotoxiticiy and apoptosis. Thienobenzocarbazoles, which have very high biological potency due to the bioisostability of pyridocarbazoles with anticancer, have great potential for CK2 inhibitors.

In Van Yüzüncü Yüzyıl University, Prof. Dr. Arif Kıvrak's research group is working on synthesis of thienobenzocarbazole derives as potential CK2 inhibitors. Druglikeness and structural properties of these molecules were investigated computationally and compared with properties of CX-4945. In addition, pharmacophore search was performed to determine their similarity with CX-4945 and protein-ligand interaction were compaired. This study provides an insight on the identification of derivatives with higher biological activity and will guide the synthesis studies.

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PP–9

Modeling and Evaluation of the Mineralization of PPCPs in Water

Evrim Arslan[1], **Başak Savun Hekimoğlu**[2], **Nilsun İnce**[2], **Viktorya Aviyente**[1]

[1]Boğaziçi University, Chemistry Department, İstanbul – Turkey
[2]Boğaziçi University, Institute of Environmental Sciences, İstanbul – Turkey

Pharmaceuticals and personal care products (PPCPs) in water are of significant environmental concern. They may result from using pharmaceutical drugs, caffeine, agricultural products or others.[1-4] Large amounts of these pollutants are detected in ground and surface water.[5] These pollutants may have toxicological effects not only on the environment but also on human health. Advanced oxidation processes are a set of chemical treatment procedures designed to remove organic materials in water by oxidation through reactions with hydroxyl radicals ($^{\cdot}$OH). The present work aims to explore the degradation byproducts of salicylic acid and methyl paraben and their toxicities to the aquatic environment. Computational tools (B3LYP / 6-31+G(d) in water) are used in order to elucidate the degradation mechanism of salicylic acid and methyl paraben. The structure-dependency degradation mechanisms of the pollutants are highlighted. Hydroxyl radical is used as an oxidant because of its strong oxidant property. The initial encounter of the pollutants with $^{\cdot}$OH is proposed to lead to either the abstraction of a viable hydrogen or the addition of the hydroxyl radical to the molecule. Both reactions are studied on different sites of the organic pollutants. Moreover, the fragmentation patterns of the molecules are investigated. Overall, the computational results are expected to interpret the experimental findings and provide theoretical support for the experimental degradation results. The calculated rates of appearance of the byproducts will guide experimentalists in their endeavor.

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PP–10

Investigation of Thermal Properties of NiO Nanopowder

Niyazi Bulut[1], Hanifi Kebiroglu[1], Bayram Gündüz[2], Tankut Ateş[1], Ömer Kaygılı[1]

[1]Fırat University, Department of Physics, Elazığ – Turkey
[2]Muş Alparslan University, Department of Science Education, Muş – Turkey

Nickel oxide (NiO) is an important transition metal oxide and its crystal system is cubic [1]. NiO has been used in various technological applications such as gas sensors, solar cells, capacitors and electrochromic films [2-4]. NiO powder with the average crystallite size of 26 nm was synthesized by a wet chemical method and its thermal properties were studied by differential thermal analysis (DTA) and thermogravimetric analysis (TGA) in the temperature range from 300 to 1150 K. It was observed that the as-produced NiO sample is thermally stable within this temperature interval. It was detected that the mass loss does not exceed the value of 1.6%.

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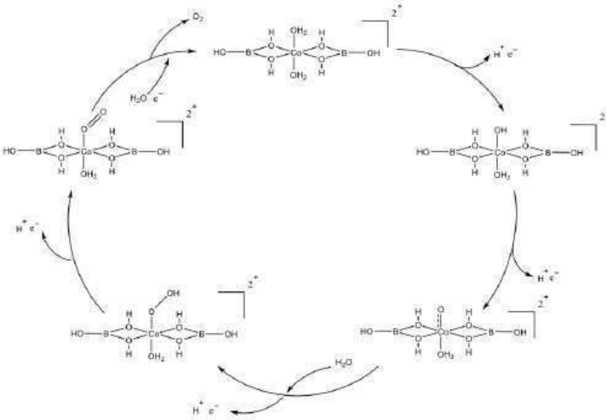
PP–11

Quantum Chemical Analysis of O–O Bond Formation at Co(IV)-Oxo Center

Ufuk Şahin, Yavuz Dede

Gazi University, Faculty of Science, Department of Chemistry, Ankara – Turkey

Search for discovery of catalysts incorporating earth-abundant materials with activities rivalling those of noble-metal catalysts in oxygen evolution reaction (OER) is peaking. [1]



Catalytic cycle of water oxidation

In this study, electrocatalytic water oxidation performance of a new cobalt-based catalyst, $Co_3(BO_3)_2$ was investigated under neutral conditions.[2] In order to gain insight into the catalytic performance of the cobalt borate system, electronic structure calculations were performed utilizing the multi-configurational Complete Active Space Self Consistent Field (CASSCF) method.

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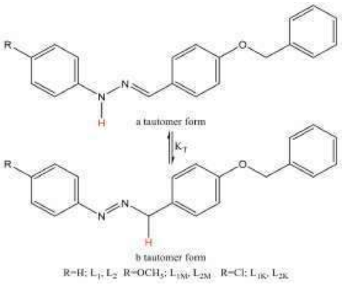
PP–12

Theoretical Calculations of Substitue Fenilhidrazin Derivate Schiff Bases

Mehmet Yıldız[1], **Halil Berber**[2]

[1]Bilecik Şeyh Edebali University & Anadolu University, Chemistry Department Common Program, Bilecik – Turkey
[2]Eskişehir Technical University, Chemistry Department, Eskişehir – Turkey

In this study, it is documented that hydrogen based on nitrogenous display tautomer forms in substitue Phenylhydrazine Derivative Schiff Bases. This causes schiff bases to show different features in solid and solvent environment. IR, UV-Vis., NMR, ...etc. particularly pose some problems in solid and solvent environments of tautomer forms in determining form. Defining tautomer ratios beforehand makes the form analysis easier. Additionally, parameters theoretically calculated such as energy, etc. shed light on severel features, including solvatokromizm, optical and electronic. Theoretical calculations of a series of synthesized beforehand substitue Phenylhydrazine Types Schiff Bases were conducted. Within the scope of this study, information on only three compounds were provided (Figure 1). These compounds and likely tautomer forms were examined and their stabilized tautomer forms were determined in the existence of vacuum and solvent, by employing DFT method B3LYP/6-311g (d,p) [1, 2, 3] level. Compound's and possible tautomer forms sum of electronic and thermal free energies (SETFE), dipole moments, mulliken charges, HOMO-LUMO energies, vibration frequencies (IR), 1H-NMR, 13C-NMR and electronic transition mechanism (UV-Vis spectrums) were calculated by means of vacuum and liquid environment.



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PP–13

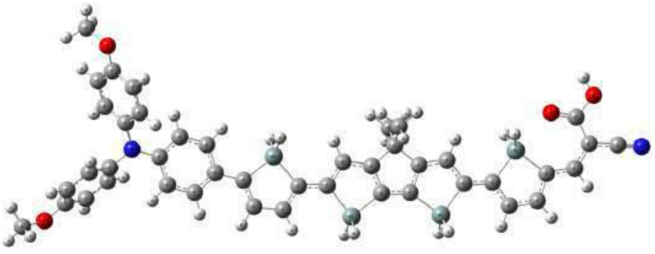
Effect of Various Parameters on the Efficiency of C226 Dyes Modified with Silicon

Merve Güreşci, Armağan Kınal

Ege University, Faculty of Science, Department of Chemistry, İzmir – Turkey

Dye sensitized solar cells (DSSCs) have become the focus of significant research efforts in recent years because of their fundamental and technological significance as new generation of solar cells. The common trend in designing dyes for use in DSSCs is based on a donor-π-spacer-acceptor (D-π-A) architecture which shows efficient intra-molecular charge transfer (ICT) properties [1]. Apart from in the D-π-A structure, the π-bridge is of great importance in tuning the energy gap and absorption properties of the dye molecule, which would significantly affect the DSSCs performance. In addition, diverse silol–containing blocks have been employed as the π-conjugated spacers of organic D-π-A dyes [2,3].

In this study, the dependence of dye-sensitive solar cell performances on various parameters namely dipole moment, electronegativity, oscillator strengths of electronic transitions, energies of frontier orbitals, conjugation and linearity was computationally investigated on new D-π-A type Si-modified-C226-dyes [4] by employing several DFT and TD-DFT methods. It is revealed that significant photon current conversion efficiency (IPCE) can be obtained depending on absorption profiles of the modified dyes.



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PP–14

A Molecular Dynamics Study of the Dmc1 Protein

Naciye Durmuş İşleyen[1,2], **Bülent Balta**[1,2]

[1]İstanbul Technical University, Department of Molecular Biology & Genetics, İstanbul – Turkey
[2]İstanbul Technical University, Dr. Orhan Öçalgiray Molecular Biology, Biotechnology & Genetics Research Center, İstanbul – Turkey

Recombinases, enzymes which generate homologous recombination, have essential roles for DNA repairing process and genetic diversity. Rad51 and Dmc1 are eukaryotic recombinases. Despite Rad51 and Dmc1 have high level sequence homology, they have different functions[1]. Dmc1 is the meiotic recombinase, plays a role in homologous recombination during crossing-over. Rad51 is crucial for DNA repair mechanism[2]. Dmc1 has two crystal structures (4HYY, 1V5W) and both of them are octameric ring structures. Some electron microscopy experiments showed that Dmc1 generates a helical filament in the presence of ATP[3].
In this study molecular dynamics simulations (MD) were performed on the Dmc1 protein in order to understand the octameric ring -helical filament transition. Protein force field ff14SB was used as implemented in the Amber14 and Amber16 packages. MD simulations were performed on the octameric ring structure of Dmc1 in the absence of DNA at different nucleotide states (ATP, ADP or nucleotide-free states). According to different nucleotide states, conformational changes of Dmc1 were determined. Different conformations were analyzed to determine whether these conformational differences have effect on the Dmc1 protein function or not.

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PP–15

Fabrication of Hole-conductor-free Mesoscopic Perovskite Solar Cells

Cesur Altınkaya[1], **Abdullah Atılgan**[1,2], **Kouroush Salimi**[2,3], **Abdullah Yıldız**[1,2]

[1]Ankara Yıldırım Beyazıt University, Faculty of Engineering and Natural Sciences,
Department of Energy Systems Engineering, Ankara – Turkey
[2]Ankara Yıldırım Beyazıt University, Central Research Laboratory Application and
Research Center, Ankara – Turkey
[3]Ankara Yıldırım Beyazıt University, Faculty of Engineering and Natural Sciences,
Department of Chemical Engineering, Ankara, Turkey

Perovskite solar cells (PSCs) have attracted great attention over the last decade due to their excellent electrical and optical properties. So far, they have demonstrated power conversion efficiencies over $\%22$ with using organic hole transport materials (HTMs) and Au counter electrodes (CEs). However, using such HTMs and CEs limits large-scale commercialization of PSCs due to their high cost and arduous synthesis routes. In this respect, hole conductor free mesoscopic PSCs have emerged as promising alternates with moderate efficiencies and low-fabrication costs. In addition, employing carbon-based CEs instead of Au is yielding highly stable PSCs against moisture and heat [1].

Here, we fabricated hole-conductor-free PSCs. $CH_3NH_3PbI_3$ perovskite was coated on mesoporous TiO_2 by using spin-coating or chemical bath deposition method. Then, carbon/graphite based CE was screen-printed on the perovskite layer. Furthermore, efficiency and characterization measurements of fabricated hole-conductor free PSCs were made by using Keithley Sourcemeter, Atomic Force Microscopy, X-Ray Diffraction, and UV-vis Spectroscopy. The results revealed that efficient, stable and low-cost PSCs were produced by carrying out all synthesis procedures under ambient environment.

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PP–16

Computational Study of Photo–oxidative Degradation of Boron Containing Oligomers

Oğuzhan Kucur[1], **Taylan Turan**[2], **Antonio Monari**[3], **Viktorya Aviyente**[1],

[1]Boğaziçi University, Chemistry Department, İstanbul – Turkey
[2]University of Basel, Department of Chemistry, Basel – Switzerland
[3]Université de Lorraine and CNRS, LPCT, Nancy – France

For the commercialization and use of a polymer-based solar cells, the stability is fundamental. Under sunlight, the performance usually deteriorates due to nanoscale morphology degradation, thermo-oxidation & photo-oxidation of the active material and electrochemical degradation of active layer materials due to the diffusion of oxygen and water through the electrode/interlayer materials.[1] Among these degradation types photo-oxidative degradation is chosen to be assessed computationally for boron containing oligomers which have been computationally studied for their optical properties by Turan et al.[2]

As these compounds contain thiophene groups in their core structure, photo-generated reactive oxygen species such as hydroxyl radical, hydroperoxyl radical, singlet and triplet oxygen's attack on these thiophene groups have been investigated. These attacks have been selected as they were previously studied for P3HT.[3] This assessment will be done in gas phase, in DCM and in acetonitrile by the help of DFT calculations to elucidate the preferred degradation mechanism of the thiophene groups in these compounds. These results will clarify the photostability, and hence the potential drawbacks of the large-scale use of this class of polythiophenes.

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PP–17

Computational Approach to the Thiol-Ene Polymerization of Natural Monomers

Hamissou Mohaman, İsa Değirmenci

Ondokuz Mayıs University, Department of Chemical Engineering, Samsun – Turkey

Recent decades, the thiol-ene polymerization process has gained special attraction due to proceeding the step-growth mechanism which results with narrow glass transitions, reduced oxygen inhibition, late gelation, and homogeneous polymer product [1,2]. The use of natural resources is developing rapidly in polymer production due to the relatively low cost and renewability of natural materials which possesses great potential as sustainable resources for the polymer industry [3]. The thiol-ene reaction mechanism of natural monomers (e.g., unsaturated fatty acids, isoprene, cinnamaldehyde) with some synthetic monomers (e.g., styrene, vinyl chloride) was investigated for the first time by quantum chemically. The structure-reactivity relationship of these monomers was elaborated to investigate their potential applications. It is well known that overall kinetics of the thiol-ene polymerization is governed by the ratio of the propagation rate constant (kp) to the chain transfer rate constant (kCT) (Figure 1). In this study, these rate constants were calculated by the transition state theory. All geometries and frequency calculations were carried out at B3LYP/6-31+G(d) level while energetics were improved by single point calculations at B3LYP/6-311++G(3df,2p) level. A good qualitative correlation obtained between experimental and theoretical results. Structure-reactivity relationships of the thiol-ene process were explained by radical stabilization energies (RSE), the charge transfer configuration and singlet-triplet gap (S-T) of substrates. Less reactivity of the conjugated systems was revealed while high reactivity of the relatively electron rich monomers were explained. Potential applications of unsaturated fatty acids by the thiol-ene polymerization processes were elaborated in this study.

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Acknowledgment We thank the Faculty of Science and Letters for the use of the Gaussian03 program package.

PP–18

Computational Investigated of Intermolecular Interactions Between Melatonin and Promazine

Tuğçe Şener Raman, Nursel Acar Selçuki

Ege University, Faculty of Science, Department of Chemistry, İzmir – Turkey

Charge transfer complexes formed by electron transfer processes act an important part of many biochemical processes. Donor-acceptor complex formation between promazine and naturally occurring hormone (melatonin) in human body at ground state were investigated using computational methods. Melatonin (MT) regulates the biological clock. Its most important function is to control many physiological and behavioral processes triggered by environmental light-darkness cycle [1]. Promazine (PZ) is a pyschotropic drug which is used extensively in mental disorders and anti-cancer activities [2]. Its interactions in metabolism with the melatonin are important in terms of its biological activity. In this study, intermolecular interactions between photophysically excited promazine and melatonin in the human body at ground-state will be investigated using computational tools. Conformational analyses have been performed to determine the initial structures for promazine and hormone (melatonin) using Spartan 08 [3]. Ground state geometry optimizations are first performed with Gaussian 09 [4] at the ω-B97XD/6-31G(d,p) level of DFT theory without symmetry constraint in gas phase and water phase, solvation calculations were performed by Tomasi's Polarizable Continuum Model (PCM) [5,6]. The electronic transitions were calculated by the time-dependent density functional theory (TD-DFT) with CAM-B3LYP, B3LYP and ω-B97XD methods using 6-311G++(d,p) basis set in gas phase and in water. Molecular orbitals, energy differences of frontier orbitals and electrostatic potentials for studied molecules were investigated. Intermolecular charge transfer between HOMO-LUMO orbitals of MT-PZ complex was observed in both media.

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PP–19

Role of chemical structure on the binding of dental adhesives

İpek Munar, Viktorya Aviyente

Boğaziçi University, Department of Chemistry, İstanbul – Turkey

Bone matrix consists of a mineral phase, hydroxyapatite (HAP) with the chemical formula of $Ca_5(PO_4)_3(OH)$ [1]. The chemical similarity of HAP and natural bone enabled to promote the research efforts in order to provide synthetic HAP as a bone substitute or surface modification agent [2]. However, the natural bone has a complex crystal structure to imitate accurately, thus the synthetic hydroxyapatites result in poor adhesion and low mechanical strength in case of dental treatments [3]. Calcium in the form of HAP is a divalent metal complex, which is used to build bone structure in mammals because of its insolubility, moreover it provides the mechanical strength to the bone. Crystal structure of calcium ions tends to bind the oxygen atoms in ligands and have the coordination number of 6 to 8 [4]. Inorganic composition of bone is unique as compared to the rest of the body, which makes HAP as a target for selective drug delivery to bone. Bisphosphonates (BPs) display high affinity to hydroxyapatite due to the structural similarity of naturally occurring pyrophosphate, therefore they can be utilized as targeting moieties [5]. The binding of BPs provided mainly by bonding of two phosphate groups to divalent calcium ion, as well as the side chain functional groups contribute to the binding affinity of the molecule [6]. Three phosphonate monomers (HAEPA, EAEPA and MAEPA) are experimentally evaluated in order to test the hypothesis that small changes in the chemical structure enhance the adhesive performance of the monomers on enamel and dentin [7]. This study investigates the binding ability of various phosphonates and bisphosphonates to divalent calcium complexes in order to model the most stable therapeutic for dental treatments by using quantum mechanical (QM) calculations.

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PP–20

Dynamics of the Homotrimeric TolC Transmembrane Protein

Işık Kantarcıoğlu, Canan Atılgan

Sabancı University, Faculty of Engineering and Natural Sciences, İstanbul – Turkey

Gram negative bacteria have two cell membranes, cytoplasmic (inner) and outer membranes between which lies the periplasmic space. Homotrimeric protein TolC which extends to the periplasm (40 Å-barrel structure embedded in outer membrane, 100 Å α-helical structure extending towards periplasmic space), is a member of outer membrane efflux protein (OEP) family. Its main role is secreting cell toxins and expulsing antibiotics. The gating mechanism of this protein has not been elucidated completely.

This study aims to probe the sub-microsecond dynamics of wild type TolC in the membrane environment whose model construction poses challenges. With this purpose in mind, the TolC crystal structure was obtained from Protein Databank (PDB ID: 1EK9) [1]. The initial orientation of the protein with respect to the bilayer was determined by utilizing the Orientations of Proteins in Membranes (OPM) database (http://opm.phar.umich.edu). The simulation box was created using CHARMM-GUI server [2]. The TolC crystal structure was placed into 256 palmitoyloleoylphosphatidylcholine (POPE) [3,4] lipid chains which is the most abundant phospholipid type in Escherichia coli. System was solvated with a minimum thickness of 15 Å TIP3[5] water molecules in each direction. Na^+ and Cl^- ions are added to mimic isotonic conditions. The CHARMM36 force field [6] was used. The prepared system was minimized for 50000 steps and equilibrated for 5 ns followed by a 100 ns production run in NPT conditions at 310 K and 1 atm using the NAMD software [7]. Our preliminary results show that the protein was stabilized within the first 10 ns of the 100 ns simulation. RMSF results indicate that the three chains of the homotrimeric TolC protein have different fluctuation profiles in the extracellular loops, despite the complete symmetry in the initial structure. In the first two dominant modes obtained via principle component analysis, [8] inward and outward motions are observed in extracellular loops and periplasmic helices at the opposite ends of the protein, while the large middle section of the protein is largely immotile. Such motions are possibly related to the picking up and disposing of the toxins by the efflux pump. Additionally, in the third dominant mode, a peristaltic motion are observed in the periplasmic helices, implicating the mechanism by which the toxins transported along the total of 140 Å distance spanned by TolC.

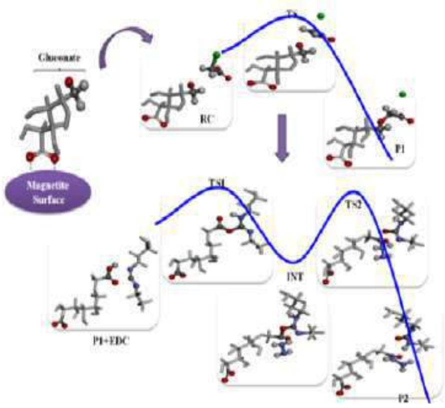
PP–21

A Computational Study on Carboxymethylation and Hydrazination Mechanisms of Gluconate

Işılay Öztürk[1], **Armağan Kınal**[1], **Güliz Ak**[2], **Habibe Yılmaz**[2], **Şenay Şanlıer**[2]

[1]Ege University, Department of Chemistry, İzmir – Turkey
[2]Ege University, Department of Biochemistry, İzmir – Turkey

Pharmacologically active anticancer drugs reach to tumor tissue with low specificity; therefore, they frequently damage healthy tissues. Nowadays, after the developments in nanotechnology, it is possible reduce harmful side effects by using nano particular drug delivery systems [1-2]. For example, when α-D-glucose coated iron oxide (magnetite) nanoparticles are loaded with an anticancer drug and it is directed to tumor tissues via an external magnetic field by mostly eliminating the side effects of classical oral treatment [3-5]. In addition, hydrazone bond formation reaction of the gluconate bound to the iron oxide surface has a highly exothermic two-step-mechanism in water. Consequently, it can be predicted that the both carboxymethylation and hydrazination reactions should be spontaneous under moderate conditions.



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PP–22

Degradation Reaction of Sulfisoxazole in Aqueous Medium by Hydroxyl Radical

Şeyda Aydoğdu, Arzu Hatipoğlu

Yıldız Technical University, Chemistry Department, İstanbul – Turkey

Sulfonamide antibiotics are used as medicine for the treatment of bacterial diseases [1]. These compounds have been used in high volumes for several decades because of their effectiveness and inexpensiveness [2]. Distribution of these compounds in the environment is a serious problem because of their potential toxicity towards to aquatic life and human health [3]. Therefore an effective elimination of them in aqueous medium is essential to protect human health. The aim of this study is to determine probable reaction path of sulfonamides degradation reactions. For this purpose sulfisoxazole was chosen as a model compound. In this work, the reaction of sulfisoxazole with hydroxyl radical have been investigated theoretically. Geometry optimizations of the reactants, the product radicals and the transition state complexes were performed with the DFT method within the GAUSSIAN 09 package. The DFT calculations were carried out using the hybrid B3LYP functional, which combines HF and Becke exchange terms with the Lee-Yang-Parr correlation functional with 6-31+g (d,p) basis set. Solvent effect was computed by using CPCM as the solvation model. The solvent was water at 25 °C, with the dielectric constant 78.39.

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PP–23

Crystallographic and 3D Morphological Analysis of ZnO Nanorods Synthesized at Different Growth Temperature

Şeydanur Kaya, Fatih Bulut, Ahmet Tolga Taşçı, Özgür Öztürk

Kastamonu University, Central Research Laboratory Application and Research Center,
Kastamonu – Turkey

Zinc oxide (ZnO) nanorod arrays were synthesized via hydrothermal route on ZnO seed layer coated glass substrate. The effect of different growth temperature (90, 120 and 150 °C) on ZnO crystal structure and morphology were investigated in detail. Crystallinity, lattice parameters and crystal size of the nanorods were determined from the X-ray diffraction. 2D surface morphology, diameter, length and aspect ratio of the nanorods were examined by scanning electron microscopy. In addition, elemental constituents were determined by energy dispersive spectroscopy mapping analysis. 3D morphological analysis of ZnO nanorods were investigated by atomic force microscopy. Also, roughness and bearing analysis were conducted from Nanoscope Analysis 1.5 software by Bruker. According to the results, a typical wurtzite crystal structure was obtained successfully in all the samples. Depending on the diffraction pattern of the samples, with increasing growth temperature, crystallinity of the samples increased. It is also seen that growth temperature has strong influence on the morphology of ZnO nanorods. With the increment in growth temperature, hexagonal nanorod structures tend to turn into pen-like structure with increased diameter.

PP–24

Optimization of CHARMM–Force Field Parameters of a Prostate Cancer Drug Enzalutamide

Sefer Baday

İstanbul Technical University, Informatics Institute, İstanbul – Turkey

Enzalutamide is the second-generation antiandrogen molecule used to treat castration-resistant metastatic prostate cancer patients. Specific point mutations on the androgen receptor can give rise to anti-cancer drug resistance. Enzalutamide can be used to treat patients where the first-generation antiandrogens fail due to key mutations [1]. Unfortunately, recently, resistance against enzalutamide has emerged in the presence of F876L mutation on the Androgen receptor [2]. The molecular mechanisms of this resistance have not been understood clearly. Molecular Dynamics (MD) simulations are powerful tools to investigate such resistance mechanisms. Insights obtained from MD simulations of receptor-ligand complex heavily depend on the quality of the parameters of the ligands. Thus, we optimized CHARMM-Force field parameters of the enzalutamide molecule.

Initial assignment of the parameters was done by using CHARMM General Force Field (CGenFF) [3]. After that, using the Force Field Tool Kit (FFTK) partial charges, bond, angle and dihedral parameters of Enzalutamide were optimized to reproduce quantum mechanics calculation results [4]. In CHARMM parameterization protocol, partial atomic charges are derived to reproduce the QM interaction with an explicit TIP3P water molecule. Water-interaction calculations were performed at HF/6–31G* level of theory to be consistent with CHARMM scheme. Bond and angle parameters were optimized using QM data obtained from Hessian calculation at the (MP2)/6–31g* level of theory. For dihedral angle optimization QM potential energy surface (PES) scans were calculated at the MP2/6–31g* level of theory.

Validation of the parameters was achieved by comparing the calculated the water-octanol partition coefficient and Infrared Spectra (IR) with the experimental data. The water-octanol partition coefficient was calculated by performing Free Energy Perturbation (FEP) calculations for enzalutamide in both water and octanol environments. IR analysis was done for the MD simulation of enzalutamide performed in water solution.

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PP–25

Electrochemical Polymerization and Characterization of Polyindene and Polypyrrole/polyindene Copolymer

Semih Danışmaz, Şadi Şen

Zonguldak Bülent Ecevit University, Department of Chemistry, Zonguldak – Turkey

This study covers the synthesis of conducting polyindene and polyindene/polypyrrole copolymer by electrochemical ways as constant potential electrolysis and cyclic voltametry. The polymers obtained in various conditions have been characterized using FT-IR Spetroscopy, Scanning Electron Microscopy (SEM), UV-vis Spectroscopy, Thermal Gravimetric Analysis (TGA), Conductivity technique. FT-IR spectrum in the spectral range of 4000-500 cm^{-1} is used to characterize the structural organization of polymer samples. The conductivities of polymers were measured by four-probe technique. Electrical conductivity of polyindene samples were found to be in the range of 10^{-6} Scm^{-1} with 10^{-5} Scm^{-1}, whereas electrical conductivity of copolymer samples found to be in the range of 10^{-3} Scm^{-1} with 10^{3} Scm^{-1}. As a result, copolymer had a beter conductivity than polyindene, due to presence of polypyrrole. Thermal stability of both two polymer types was investigated by thermogravimetric analysis. Thermal degradation temperature and residue are observed from thermogravimetric curves, ranged from 20 °C to 800 °C. SEM image of polyindene samples show granular structures, while SEM image of copolymer samples show cauliflower structure. UV-vis spectra of samples was taken to have an idea about electrochromic properties. Some related properties of polymer samples mentioned above were examined depending on some parameters such as temperature, electrolysis period, concentration, applied potential etc.

PP–26

A Computational Study on Reaction of Dimethylmalonate Addition to trans--Nitrostyrene with New Approach

Sezen Alsancak, Yeşim Çamlısoy, Nihan Çelebi Ölçüm

Yeditepe University, Department of Chemical Engineering, İstanbul – Turkey

Quantum mechanical calculations have successfully uncovered numerous organocatalytic reaction mechanisms and explained the observed reaction outcomes; yet, study on highly complex multifunctional organocatalysts is still a challenging task due to the large number of conformational degrees of freedom. Proposed new computational approach [1] that combines the quantitative power of quantum mechanical calculations with drug design tools provides an opportunity to explore activities and selectivities of complex multifunctional organocatalysts for a target reaction. This work will describe how the quantitative power of quantum mechanical calculations is coupled with drug design tools to shed light on the ambiguous active conformations and mode of action of 2-aminoDMAP/urea catalysts and explain the origin of catalysis in the dimethyl malonate addition to trans--nitrostyrene (Scheme 1). To understand the elements responsible for catalytic mechanism and selectivity of the target reaction, the catalytic active site models were generated using quantum mechanical calculations. The functional groups of complex multifunctional organocatalyst determined as pharmacophore groups. Catalytic group maps were generated using arrangement of these pharmacophore groups in the active site models. The resulting catalytic group maps were screened against a conformational library generated for complex multifunctional organocatalyst. Thus, organocatalysts with the desired three-dimensional arrangement of catalytic functional groups were determined. The ambiguous active conformations and mode of action of multifunctional organocatalysts with complex structures were demonstrated.

1. Tübitak 1001, 'Determination of Active Organocatalysts Using Computational Methods', 114Z791

PP–27

Effects of Environment on DNA’s Structure and Electrical Conductivity

Sümeyye Gökce[1,2], **Büşra Demir**[1,2], **Hashem M. Mohammad**[3], **Sunil R. Patil**[4],
M. P. Anantram[3], **Ersin Emre Ören**[1,2]

[1]TOBB University of Economics & Technology, Department of Biomedical Engineering,
Bionanodesign Laboratory, Ankara – Turkey
[2]TOBB University of Economics & Technology, Department of Materials Science and
Nanotechnology Engineering, Ankara – Turkey
[3]University of Washington, Department of Electrical Engineering, Seattle, WA 98195, USA
[4]Pune, College of Engineering, Department of Physics, MS – India.

Molecular electronics is the design and manufacture of electronic devices using molecular building blocks such as DNA/RNA/peptides and their hybrids with nanomaterials. This research area is expected to provide the necessary resources to extend Moore’s Law beyond the foreseen limits of small-scale conventional silicon integrated circuits. Understanding of the electronic band structures and electron transport mechanisms of many different molecular systems is necessary to build new molecular devices. DNA is a promising molecule for molecular electronics based on its unique electronic and self-assembly properties. In order to control DNA conductance, its electronic properties have been studied over the years both theoretically and experimentally. However, conformational, chemical and environmental factors have an important effect on controlling conductance of DNA and make this problem interesting. DNA has several conformations under different solvent conditions. A and B DNA are two of them that are thought to exhibit different electrical properties. In this study, to analyze the effect of environment on conformations of DNA, we first completed Molecular Dynamics simulations and determined the A-B transformation path. After that we chose representative structures from the simulations and analyzed the electronic properties of the structures using Density Functional Theory. Our results show that environmental differences may be used to control both the conformation and thus the conductance of the DNA for future electronic devices.

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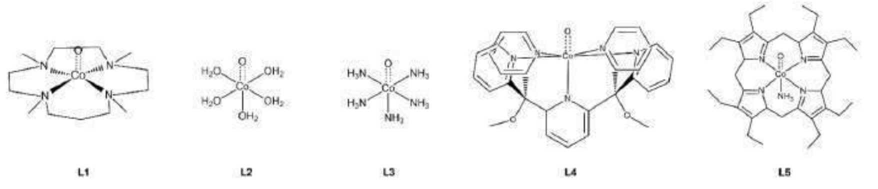
PP–28

On the Electronic Structure of Co(IV)-O Complexes

Muhammed Büyüktemiz, Osama Qandeel, Yavuz Dede

Gazi University, Faculty of Science, Department of Chemistry, Ankara – Turkey

High valent Metal–oxo complexes are proposed as key reactive intermediates in a variety of important oxidative transformations.[1] Direct evidence of early transition metal (TM) complexes featuring an -oxo moiety are abundant. For late TM complexes however, occupied π^* orbitals result in, unstable M–O bonds hence non-elusive species that are intriguing from perspectives of reactivity and electronic structure. Recently, an interesting electronic structure fingerprint in penta-coordinated Co(IV)–O environments was identified.[2-4] The MOs primarily involved in the Co–O bonding are the fully occupied low lying (Co–O) σ and (Co–O) π and two half-filled (Co–O)π^* antibonding orbitals. The result was an unusual $|\mathrm{Co(d)}(\uparrow)\rangle$ $|\mathrm{Co(d)}\pm\mathrm{O(p)}(\uparrow)\rangle$ $|\mathrm{Co(d)}\pm\mathrm{O(p)}(\uparrow)\rangle$ electronic configuration in an overall quartet (S = 3/2) coupled fashion.



Species studied in this work

Herein, we report such an unusual electronic configuration is persistent in variety of Co(IV)–O complexes that are employed particularly for catalytic oxidation among many other important chemical transformations.

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PP–29

Network Analysis of Point Mutations That Induce Ligand Switching in PDZ Domains

Tandaç Furkan Güçlü, Nazlı Kocatug, Canan Atılgan

Sabancı University, Molecular Biology, Genetics and Bioengineering, İstanbul – Turkey

Point mutations occasionally change protein structure and/or function, and with these changes, important alterations in ligand specificity [1] that have consequences, e.g. in antibiotic resistance [2] may occur. Here we study the PDZ domains which construct different complexes by binding various of ligands; they have an important role in cell signaling. Previously, PDZ domains have been demonstrated to have ligand specificity which switches between two ligands when G330T and/or H372A mutations are inserted [1]. The wild-type (WT) protein prefers binding to ligand I, and the G330T mutation binds to both ligand I/II while the H372A mutation and the G330T-H372A double-mutation tend to bind only to ligand II. To understand the resiliency of residues against mutational perturbances, we utilized the WT protein structure and mutated each residue to alanine. Then, we conduct network analysis on each structure and calculated the network measures with a focus on the average path length (L) and betweenness centrality (BC), as the former characterizes the overall accessibility of each node, and the latter demonstrates the central nodes which control the information flow in a residue network [3–5]. Furthermore, 200 ns-long molecular dynamics (MD) simulations of the apo form of the four variants were investigated. We monitor the network measures throughout the trajectories and compare the results to the single point values obtained from the earlier alanine mutation scan. Our results show that L values of the residues at the N terminus and BC values of the residues at the C terminus get lower when bound to ligand II. These slight changes of the residue centralities by perturbations introduced in the form of mutations lead to the ligand switching behavior in the PDZ domain. We conclude by discussing how the network measures may be associated with thermodynamic variables that contribute to binding.

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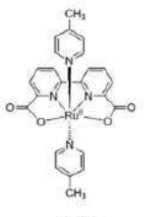
PP–30

Computational Study of Ruthenium Based Water Oxidation Catalysts

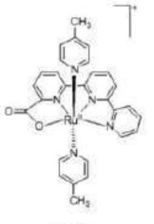
Öyküm Naz Avcı[1], **Mariachiara Pastore**[2], **Antonio Monari**[2], **Şaron Çatak**[1]

[1]Boğaziçi University, Chemistry Department, İstanbul – Turkey
[2]Université de Lorraine and CNRS, LPCT, Nancy – France

Water oxidation is a critical step of the solar-driven water splitting to produce hydrogen, which is one of the best strategies for the production of clean and renewable energy to cover the increasing societal demand. The need for an effective water oxidation catalyst (WOC) is necessary to overcome the reaction slow kinetics also due to the high number of electon/proton transfer and the large overpotential. Molecular transition metal based WOC have been extensively studied, due to their structural simplicity, synthetic versatility and the simpler mechanistic investigation.[1] Two different water oxidation mechanisms are usually invoked: i) water nucleophilic attack (WNA) on a single metal complex and ii) the oxidation driven by the formation of a two metal center (I2M). [2] Two ruthenium based water oxidation catalysts that share structurally similarities but showing different trend, experimentally studied by Fan et al. [3], are selected to evaluate their mechanistic properties.
Computational comparison of the reaction mechanistic cycles for the two mononuclear ruthenium based catalysts are investigated in order to understand which factors can affect their reaction pathways and in particular favor one of the two mechanisms. Our study, rationalizing, at DFT level, the geometrical and electronic factors driving the full water oxidation cycle will help to understand the structure/activity relationships.



Ru-bda



Ru-tpc

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PP–31

The Effect of $CH_3NH_3PbI_3$ Perovskite on Dye–sensitized Solar Cells Performance

Abdullah Atılgan[1,2], **Cesur Altınkaya**[1], **Kouroush Salimi**[2,3], **Abdullah Yıldız**[1,2]

[1]Ankara Yıldırım Beyazıt University, Faculty of Engineering and Natural Sciences,
Department of Energy Systems Engineering, Ankara – Turkey
[2]Ankara Yıldırım Beyazıt University, Central Research Laboratory Application and
Research Center, Ankara – Turkey
[3]Ankara Yıldırım Beyazıt University, Faculty of Engineering and Natural Sciences,
Department of Chemical Engineering, Ankara, Turkey

Dye-sensitized solar cells (DSSCs) have been extensively studied by many researchers since the first report was published by Gratzel in 1991. The low fabrication cost, non-toxicity and enabling flexible structure designs have been superior features of DSSCs [1,2]. However, their moderate efficiencies compared to conventionally used Si-based solar cells and stability issues remained unsolved challenges till today. On the other hand, using perovskite-based materials in solar cell applications have demonstrated promising power conversion efficiencies over the last decade. Therefore, incorporation perovskite materials with DSSCs can open a new avenue to enhance the efficiency of DSSCs.

In this work, we report the synthesis and efficiency studies of N719 dye $CH_3NH_3PbI_3$ perovskite incorporation as an additive sensitizer in DSSCs. Fluorine doped tin oxide (FTO) glass was immersed in a low molarity titanium tetrachloride aqueous solution. Dense and mesoporous TiO_2 layers were coated on FTO glass using spin coating technique to obtain photoanodes (PAs). After PAs were immersed in N719 dye solution, CH3NH3PbI3 perovskite deposition was carried out on N719 dye loaded PAs. Pt/FTO glass counter electrodes (CEs) were prepared, and with adding drops of electrolyte solution between PAs and CEs, assembling of DSSCs was completed. Furthermore, the crystal structure and optical absorbances of PAs were measured by means of XRD and UV-vis Spectroscopy, respectively. The surface morphologies of PAs were analyzed by Atomic Force Microscope (AFM) in non-contact wave mode before dye loading. The photocurrent-voltage (I-V) characteristics of the DSSCs were carried out by a computer controlled Keithley 2400 Sourcemeter. The results revealed that efficient and low-cost DSSCs can be obtained by using $CH_3NH_3PbI_3$ perovskite as an additive sensitizer.

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PP–32

Theoretical Investigation of Electronic Properties of the Ethylenedioxyselenophene Containing Donor-acceptor-donor Type Conjugated Polymer

Özge Özkılınç, Hakan Kayı

Ankara University, Chemical Engineering Department, Computational Chemical
Engineering Laboratory, Ankara – Türkiye

Conjugated polymers have attracted researchers, since semiconducting polymers have light weight, they are cost effective and can be used as flexible electrode materials. In this study, quantum chemical calculations are carried out by the help of density functional theory (DFT) to calculate the HOMO (highest occupied molecular orbital) - LUMO (lowest unoccupied molecular orbital) energy gap. Investigated conjugated polymers chosen as 4,7-di(selenophen-2-yl)benzo[c][1,2,5] thiadiazole and 4,7-bis(2,3-dihydro-seleno[3,4-b]-1,4-dioxin-5-yl)benzo[2,1,5]-thiadiazole. Electronic properties adjusted by designing the molecular structure of the starting monomer to obtain a better control over the band gap values (Eg) by using “donor-acceptor-donor (D-A-D) method". Conformational analysis was done by using Density Functional Theory utilizing the B3LYP (Becke three-parameter hybrid correlation functional combined with Lee-Yang-Parr correlation functional) method with LANL2DZ basis set. The theoretical methods used in this study are promising for the modelling of similar D-A-D type novel conjugated polymers.

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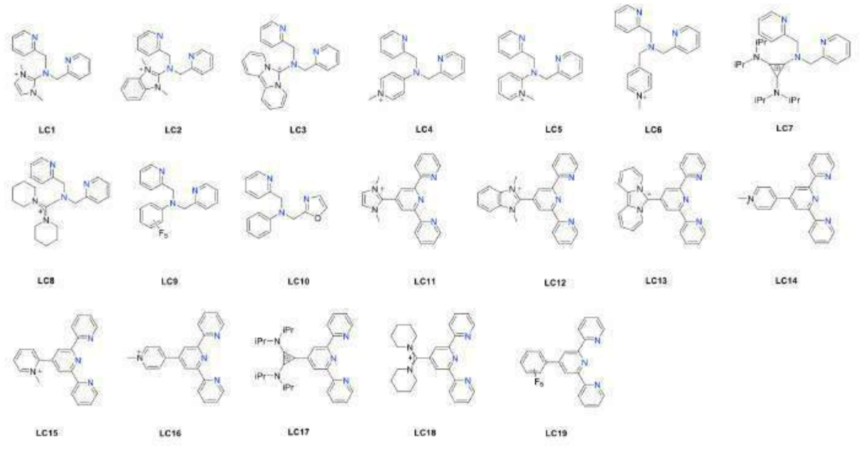
PP–33

Oxidative Methane Activation With Cationic Ligand-metal Complexes

Yıldız Ocak, **Yavuz Dede**

Gazi University, Faculty of Science, Department of Chemistry, Ankara – Turkey

Oxidative C–H bond activation is of utmost importance in the context of converting small hydrocarbons to alcohols as an alternative to fossil fuel consumption.[1] Despite decades of continued research that utilized transition metal compounds, only a limited number of simultaneous O_2 and C–H activation processes are available.[2,3] It is still an immense challenge to convert methane into methanol by using low cost catalysts under mild conditions. Herein, the C–H activation reactions by theoretically designed cationic ligand - transition metal complexes were studied with quantum chemical methods based on density functional theory (DFT). Barriers of hydrogen atom transfer step in methane activation with different ligand environments (Figures 1) were reported.



Cationic ligands investigated in this study. Nitrogen atoms coordinating to the metal (Fe(II), Cr(II), Mn(II), Ni(II), Co(II)) are shown in blue

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Acknowledgment TUB0130TAK (project number: 117Z337) is gratefully acknowledged for financial support.

PP–34

Click Chemistry in the Presence of S-containing Ligands

Gülbahar Bozan, Nurcan Şenyurt Tüzün

İstanbul Technical University, Department of Chemistry, İstanbul – Turkey

Azide-alkyne cycloaddition reaction (CuAAC) in the presence of a copper catalyst is a prototype reaction of click chemistry approach. From the reaction of azides and alkynes, 1, 2, 3-triazoles are synthesized effectively and regioselectively at convenient conditions. Most of the starting alkynes and azides are commercially available and many others can be synthesized with functional groups and their cycloaddition reaction with copper as catalyst selectively gives 1,2,3-triazoles under aqueous conditions, even at room temperature. Furthermore, the CuAAC reaction is quick; it can take place with a wide range of substrates and shows tolerance to reaction conditions. As a part of continuous effort from our laboratory, the mechanism of CuAAC reaction has been investigated by quantum mechanical calculations. In this study, DFT calculations have been performed to investigate the ligand effect on the reaction by adding various sulfur-based ligands on Cu metal in the synthesis reaction of 1-Sulfonyl-1, 2, 3-triazoles. The mechanism for CuAAC reaction has been modelled with quantum mechanical calculations by considering the previous experimentally and computationally proposed pathways. Five different sulphur-based ligands with good and poor yields have been chosen to comprehend the differences between the structures by performing calculations on the proposed pathways. Understanding the mechanism in detail can enable one to make more efficient synthesis with desired functional groups. For this purpose, DFT functionals such as M06-L functional has been utilized in calculations performed with Gaussian 09 software with 6-31+G (d,p) basis set.

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PP–35

Determination of the Effects of Electronic Properties of Several Metal-containing Initiator Complexes on Polymer Molecular Weights in the Ring Opening Polymerization of δ–valerolactone: A Computational and Experimental Study

Sıla Gümüştaş, Armağan Kınal

Ege University, Department of Chemistry, Faculty of Science, İzmir – Turkey

Poly(δ-valerolactone), PVL, synthesized by ring opening polymerization (ROP), is an attractive polymer with good biodegradability, biocompatibility, and hydrolyzability properties. A large variety of metal complexes containing alkyl, alkoxide, carboxylates and oxides, which are used as initiators, have been reported to possess good activity [1]. Electrophilicity of metal center located at initiator plays an important role in the ring opening polymerization of cyclic lactones since it attracts oxygen atom of carbonyl group of cyclic lactone [2]. In addition, the metal complex having the lowest energy LUMO among the metal-containing initiators used in polyester synthesis has a greater tendency to make bond with the carbonyl oxygen in the monomer3. Thus, determination of atomic charges on metal centers (via NBO analysis) are taken into account together with LUMO energy comparisons of initiator complexes (LUMO analysis) might help choosing a good initiator. In this study, stable structures and atomic charges on metallic centers (via NBO analysis) of $SnAcet_2$, $PbAcet_2.3H_2O$, $CdAcet_2.2H_2O$, $NiAcet_2.4H_2O$ and $CuAcet_2.H_2O$ complexes that can be used as initiators for PVL synthesis were computationally determined with several DFT methods. It is revealed that the molecular weight differentiations of the PVLs that were synthesized with aforementioned initiators can be explained by the joint evaluation of NBO and LUMO analyzes. Therefore, these analyses can help to discover a good initiator leading to a high molecular weight polymer.

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PP–36

Electronic Properties of Penicillin Derivaties

Şeyda Aydoğdu, Nesrin Işıl Yaşar, Buse Süleymanoğlu, Arzu Hatipoğlu

Yıldız Technical University, Chemistry Department, İstanbul – Turkey

Antibiotics are essential for the public health and life quality. However depend on the usage in large quantities they pose serious risks for human and animal health. They have also been found over the last 20 years as microcontominants in soil and water ecosystems. When antibiotics occur in the environment, they can hamper microbial community structure and provoking serious health problems [1,2]. Therefore, antibiotics need to be removed from the environment.

Penicillins are antibiotics used to treat bacterial infections such as pneumonia, uncomplicated gonorrhea, meningitis and other serious infections [3]. In this study, the structures of 4 penicillins namely penicillin V, penicillin G, methicillin and ampicilin were investigated theoretically. Molecular descriptors were determined with the intention of predicting the degradation reactions of penicillins. Conformational analyses and geometry optimizations of all the structures were performed to determine the most stable structures. All of the molecules were modelled with DFT at B3LYP/6-31G* level in Gaussian 09W program package. The solvation effects were computed using CPCM as the solvation model. The electronic energies, electron densities, molecular charge distributions of the molecules and the DFT reactivity descriptors such as chemical hardness, electronegativity and electrophilicity index for all the molecules were calculated.

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PP–37

Investigation of Ozonolysis of Unsaturated Acids by Computational Tools

Sulaiman Mohammed Sulaiman Qaroot[1], **Cenk Selçuki**[2]

[1]Ege University, Graduate School of Natural and Applied Science, Biochemistry Department, İzmir – Turkey
[2]Ege University, Faculty of Science, Biochemistry Department, İzmir – Turkey

Ozonolysis is described as the reaction of ozone with unsaturated carbon-carbon double bonds. The reaction may take place in gas phase as well as in aqueous phase. It is one of the reactions used in organic synthesis. Additionally, it is one of the reactions used to degrade the pollutants in water environment. Current study investigates the ozonolysis reactions of fumaric, malic acrylic and methacrylic acids in gas and aqueous phases. The calculations will be carried out at B3LYP/6-311++G(d,p) level as implemented in Gaussian16 [1]. Structures, electronic and thermodynamical properties of all studied systems will be investigated by using both concerted and stepwise reaction mechanisms.

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Acknowledgment Calculations were performed on FenCluster (Ege University Faculty of Science) and on TUBITAK-ULAKBIM Truba resources.

PP–38

Proton Transfer in Sulfur Containing Methanethiol Clusters: An Experimental and Theoretical Studies

Nevin Uras–Aytemiz[1], **F. Mine Balcı**[2], **J. Paul Devlin**[3]

[1]Karabük University, Department of Chemistry, Karabük – Turkey
[2]Süleyman Demirel University, Department of Chemistry, Isparta – Turkey
[3]Oklahoma State University, Department of Chemistry, Stillwater, OK – United States

HCl solvation on/in methanethiol nanoparticles at low temperatures was investigated by FTIR spectroscopy and ab initio molecular dynamics as implemented in the density functional code QUICKSTEP (which is part of the CP2K package) [1,2]. Some of the results have been further checked with MP2 level calculations by Gaussian 09 package program [3]. Unlike the HCl-CH_3OH system, which has been examined before [4,5], HCl on the surface or within methanethiol nanoparticles does not achieve an ionized form. The non-covalent interactions (NCI) [6], atoms in molecules (AIM) [7] and DFT–SAPT (symmetry adapted perturbation theory) calculations within Molpro program [8] were applied to some of the S-containing and O-containing clusters in order to get additional insight of the nature of the interactions.

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Acknowledgment This work was supported by TUBITAK (Project No: 105T234)

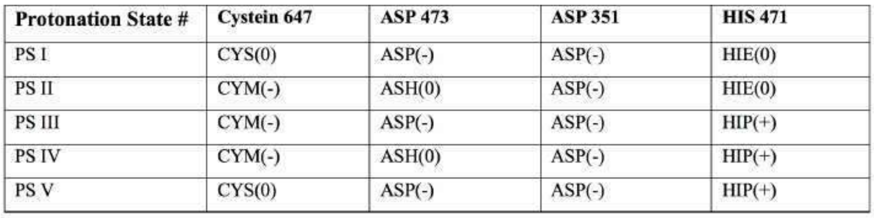
PP–39

Multiscale Study to Elucidate the Reaction Mechanism of Protein Arginine Deiminase 2

Fethiye Aylin Sungur[1], **Sinan Başçeken**[2], **Erdem Çiçek**[1] **Gerald Monard**[3],
Viktorya Aviyente[4]

[1]İstanbul Technical University, Informatics Institute, İstanbul – Turkey
[2]Hitit University, Chemistry Department, Çorum – Turkey
[3]Boğaziçi University, Chemistry Department, İstanbul – Turkey
[4]Université de Lorraine, Vandoeuvre-les-Nancy – France

Protein Arginine Deiminase (PAD) enzymes catalyze the citrullination reactions from post-translational modifications of histones [1]. It has been experimentally determined that PAD2 from five different PAD enzymes identified in the human body has a role in uncontrolled growth of ER+ type breast cancer cells. The three-dimensional structure of PAD2 h identified recently. PAD2 reported to catalyze the citrullination reaction by a substrate-assisted mechanism, unlike other members of the family. To best our knowledge, a computational study on the mechanism and the dynamic behavior of PAD2 has not been performed yet. It has been stated that the PAD active site contains a Cys-His catalytic dyad (Cys647 and His471 in PAD2). In addition, PAD2 contains two aspartyl residues (Asp351 and Asp473) that position the guanidinium group for the nucleophilic attack by the active site cysteine. Based on pKa results we have proposed different protonation states for selected residues (Table 1). We generate the QM and MD models based on those protonation states. Beside the experimentally proposed one, several alternative mechanisms were studied at M062X/6-31+G (d,p) level of theory in order to get a deeper understanding of the mechanistic insights of the reactivity.



Protonation State #	Cystein 647	ASP 473	ASP 351	HIS 471
PS I	CYS(0)	ASP(-)	ASP(-)	HIE(0)
PS II	CYM(-)	ASH(0)	ASP(-)	HIE(0)
PS III	CYM(-)	ASP(-)	ASP(-)	HIP(+)
PS IV	CYM(-)	ASH(0)	ASP(-)	HIP(+)
PS V	CYS(0)	ASP(-)	ASP(-)	HIP(+)

Table 1: Possible protonation states for the selected residues

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PP–40

Energetics of Ion Transfer Through Open Sodium Channel NaVMs

Murat Çavuş[1], **Esra Körpe**[2], **Serdar Kuyucak**[3], **Turgut Baştuğ**[2,4]

[1]Yozgat Bozok University, Department of Science Education, Yozgat – Turkey
[2]TOBB University of Economics & Technology, Micro and Nanotechnology Graduate Program, Ankara – Turkey
[3]University of Sydney, School of Physics, Sydney – Australia
[4]Hacettepe University, Faculty of Medicine, Department of Biophysics, Ankara – Turkey

Voltage-gated sodium (Nav) channels initiate and propagate action potentials in excitable cells. Mutations in these channels are responsible for a variety of disorders, including epilepsy and pain syndromes. Therefore, they are the target of a number of drugs used for reducing pain and seizures. In this study, we investigate ion permeation in an open NaVMs channel by performing molecular dynamics simulations and potential of mean force calculations. In simulations, Na^+ ions are observed to enter the channel from bulk but not from the cytoplasm. Even after loading the channel with extra Na^+ ions, they are observed to exit only to the bulk side. To understand the energetics of this behavior, we have constructed potential of mean forces for the exit of a Na^+ ion when the filter is occupied by 1, 2 and 3 Na^+ ions. In all cases, a substantial energy barrier is found at the intracellular gate, where hydrophobic residues form a narrow neck and prevent passage of a fully hydrated Na^+ ion. Our results indicate that for conduction of Na^+ ions either the gate needs to be somewhat more open or the hydration number of Na^+ should be marginally lower than that predicted by the current force fields.

Acknowledgment Simulations were performed at the ULAKBIM cluster of TUBITAK (Ankara). This work was supported by the Scientific and Technical Research Council of Turkey (TUBITAK Grant No. 115Z505) and Yozgat Bozok University (Scientific Research Projects Nos. 6602c-EF/16-19).

PP–41

Calculating by B3LYP/6-31G(d) of the theoretical electronic absorption spectra of KD dyes in vacuum and solvent

Nermin Kutlu

Süleyman Demirel University, Physics Department, Isparta – Turkey

Dyes normally don't have particle size. A particle of dyes is also thought of as an agglomerate in solvents. The deviations in absorption spectra can arise from inhomogenous dye molecules which have aggregation structure at especially between 10^{-3} – 10^{-6} M concentrations in solution phases. In this study, the optimized geometries, electronic structures and electronic absorption spectras of KD dyes were calculated by DFT/TD–DFT at B3LYP/6-31G* basis set using the Gaussian 09 program in vacuum and solvent. According to theoretical calculating results, KD dyes have the aggregate structure at $5\text{x}10^{-5}$ M concentration in chloroform solvent.

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PP–42

Computational Investigation of Interactions Between Hydroxyproline and Chromium Complexes

Nursel Acar Selçuki[1], **Deniz Kalender**[2]

[1]Ege University, Faculty of Science, Department of Chemistry, İzmir – Turkey
[2]Ege University, Faculty of Science, Department of Leather Engineering, İzmir – Turkey

Chrome among mineral tanning materials is the most widely used tanning material, accounting for more than 80% of all produced leather products. Amino acids contain amine (-NH_2) and carboxyl (-COOH) groups and a side chain except glycine. Coordination of protein carboxyl groups to chromium is the main reaction in chrome tannage. Calculations were carried out using Density Functional Theory (DFT) at B3LYP 6-311++G(d,p) level. For metals LANL2DZ basis set was used. Excited state calculations were carried out with Time-Dependent Density Functional Theory (TDDFT) at the same level using the first 100 singlet excitations. Orbital energies, UV-Vis spectra, and total electron densities were shown for gas phase. All calculations were performed using Gaussian094. Calculations reveal that hydroxyproline and chromium form stable complexes in water.

1. Gaussian09 Version C.01 (2009) M. J. Frisch et al. Gaussian, Inc., Wallingford CT.

Acknowledgment Quantum chemical calculations were performed using FenCluster (Ege University Faculty of Science) and TUBITAK-ULAKBIM Truba resources.

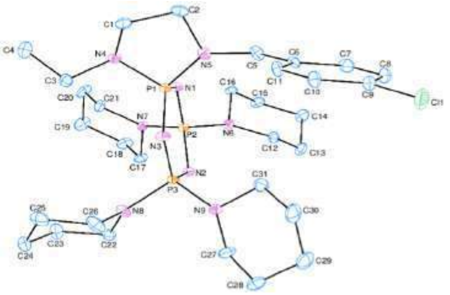
PP–43

Crystal Structures and Spectroscopic Properties of Partly- and Fully-substituted Monospirocyclotriphosphazenes

Nuran Asmafiliz[1], **İpek Berberoğlu**[1], **Zeynel Kılıç**[1], **Tuncer Hökelek**[2]

[1]Ankara University, Department of Chemistry, Ankara – Turkey
[2]Hacettepe University, Department of Physics, Ankara – Turkey

Hexachlorocyclotriphosphazene (trimer), $N_3P_3Cl_6$, has been a useful molecule for the preparation of the substituted phosphazene frameworks with mono-, di-, tri-, and tetra- functional reagents [1,2]. The condensation reaction of hexachlorocyclotriphosphazene, $N_3P_3Cl_6$, with N-ethyl-N-mono(p-chloro-benzyl)-ethanediamine, $ClPhCH_2NH(CH_2)2NHC_2H_5$, produce new tetrachloro monospirocyclotriphosphazene. After that, the fully-substituted phosphazene derivatives are obtained from the reactions of the partly-substituted tetrachloro compound with monodentate secondary amines [pyrrolidine, morpholine, piperidine, 1,4-dioxa-8-azaspiro[4,5]decane (DASD)]. The structures of the partly and fully-substituted phosphazenes are determined using elemental analyses, FTIR and mass spectra, and the obtained NMR spectral data from the one-dimensional (^{1}H, ^{13}C and ^{31}P NMR) and two-dimensional (HSQC ve HMBC) NMR techniques. The molecular and solid state structures, the conformations of the phosphazene rings and the substituents of the two phosphazene compounds are determined using X-ray diffraction techniques.



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PP–44

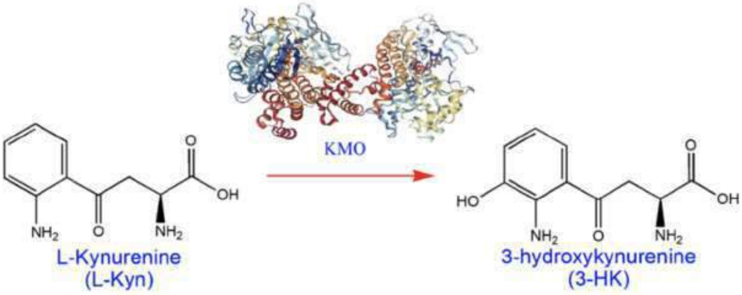
Quantum Cluster Approach to the Hydroxylation Reaction in the Presence of KMO Enzyme

Nurcan Ş. Tüzün, Yılmaz Özkılıç

İstanbul Technical University, Department of Chemistry, İstanbul – Turkey

In this DFT study we explore the mechanism of KMO (kynurenine 3-monooxygenase) catalyzed hydroxylation reaction between substrate Kyn (L-Kynurenine) and FAD (flavin adenine dinucleotide) with the application of quantum-cluster approach. The illumination of the mechanism of this enzymatic reaction is very important since it holds the potential to expose therapeutic information about the malfunctioning KMO catalysis which known to cause several diseases like Alzheimer's and Parkinson's or disorders like bipolar and schizophrenia.

According to the results obtained from these calculations, initially the hydroxyl in the flavin hydroperoxide intermediate is transferred to Kyn with an electrophilic aromatic substitution. The barrier of this step is reduced with the proline residue which allows the stabilization of the charge of hydroxyl moiety being transferred. The following hydride transfer takes place rapidly yielding the stable keto 3-HK (3-hydroxykynurenin) intermediate. To proceed in the forward direction, with a reasonable rate, the third transformation requires reorganization of the hydrogen bonding network around the substrate to initiate a water assisted tautomerization giving the product 3-HK. In the final step FAD returns to its oxidized state with a dehydration transition state which is achieved with the participation of 3-HK as a catalyst and a water molecule. In calculations, 348 atoms from the active site were included. The optimizations and the frequency calculations of the structures obtained with the quantum cluster scheme were performed at the B3LYP/6-31G(d,p) level and their single point calculations were performed at the B3LYP/6-311+G(2d,2p) level with dielectric constant=4.



PP–45

Crystallographic Characterizations of Cis- and Trans-dispirocyclic Ferrocenylphosphazenes

Yasemin Tümer[1], **Nuran Asmafiliz**[2], **Zeynel Kılıç**[2], **Tuncer Hökelek**[3]

[1]Karabük University, Department of Chemistry, Karabük – Turkey
[2]Ankara University, Department of Chemistry, Ankara – Turkey
[3]Hacettepe University, Department of Physics, Ankara – Turkey

Novel cis- (4-6) and trans-dispirocyclic ferrocenylphosphazene derivatives (7-9) were obtained by reactions of hexachlorocyclotriphosphazene with N-alkyl-N-monoferrocenyldiamines of the formula $FcCH_2NH(CH_2)nNHR$ [n = 2, R = CH_3 (1); n = 2, R = C_2H_5 (2) and n = 3, R = CH_3 (3)] [1]. The crystal structures of 5 (with 8), 6, 7 and 9 were determined by X-ray crystallography (Fig. 1 and 2). The most important result of this study was that the trans chiral phosphazenes crystallized as only one enantiomer.

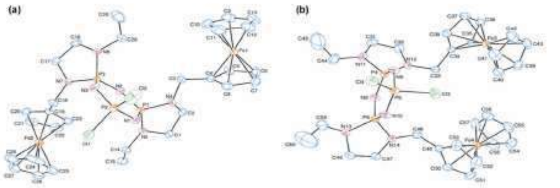


Figure 1: ORTEP-330 drawings of (a) 5 (cis) and (b) 8 (trans) with the atom-numbering schemes. Displacement ellipsoids are drawn at the 30% probability level.

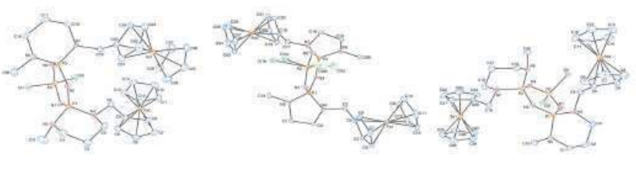


Figure 2: ORTEP-330 drawings of 6, 7 and 9 with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level

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PP–46

Reactions of Azinphos-methyl Pesticides: A Quantum Mechanical Study

Yelda Yalçın Gürkan, Bahar Eren, Selim Özgür

Tekirdağ Namık Kemal University, Department of Chemistry, Tekirdağ – Turkey

Azinphos-methyl they have high volatility, they are of great environmental interest. They cause severe health problems. In recent years, due to their carcinogenicity and mutagenicity, quantum mechanical studies on their removal from air and water have gained a considerable interest.

This study aims to predict degradation mechanism of azinphos-methyl molecule in gas phase and aqueous media. The probable reaction path of azinphos-methyl molecule with OH radical have been analyzed. The optimized geometry was calculated via Gauss View 5. Subsequently, the lowest energy status were found out through geometric optimization via Gaussian 09 programme. With the aim to determine the intermediates occurring at the photocatalytic degredation mechanism of hetacillin, geometric optimization of molecule was realized through Density Functional Theory (DFT) method. Activation energy for probable reaction path was calculated, and their most stable state from the thermodynamic perspective for the gas phase and aqueous media. The impact of water solvent was investigated by using COSMO as the solvation model. The predicted mechanism was confirmed by comparison with the experimental results on simple structures reported in the literature.

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Acknowledgment The authors greatly appreciate Namik Kemal University Research Foundation for financial support. Project number: NKUBAP.01.GA.18.164

PP–47

Physical properties and Chemical Analysis of Phases of NiMnSnCr Shape Memory Alloy

Zehra Deniz Çırak[1], **Mediha Kök**[2], **Şeyda Burcu Durğun**[2], **Ayşe Aydoğdu**[3]

[1]İnonü University, Health Services Vocational School, Malatya – Turkey
[2]Fırat University, Department of Physics, Elazığ – Turkey
[3]Gazi University, Department of Physics, Ankara – Turkey

In this study, Thermal and magnetic properties of NiMnSnCr shape memory alloys were determined as a physical properties by using Differential Scanning Calorimetry (DSC) and Physical Properties Measurement Systems (PPMS) device. The crystal structure and microstructure analyses on NiMnSnCr alloys were done by using x–ray diffraction (XRD) and scanning electron microscopy (SEM). It was seen that there are two phases in microstructure of NiMnSnCr alloys. These phases named as martensite and gamma phase. The phase's chemical compositions are determined by energy dispersive X–ray spectroscopy (EDX). It was found that the gamma phase ratio was found to be increased by chromium addition in NiMnSnCr alloys.

Acknowledgment This work was supported by Inonu University BAP (Project number:TSA-2017-871)

PP–48

A Computational Study on Tri and Tetraazaanthracenes

Zeynep Turhan İrak[1], **Ahmet Köle**[2], **Selçuk Gümü**[1,3]

[1]Iğdır University, Iğdır – Turkey
[2]Van Yüzüncü Yıl University, Van – Turkey

Tri and tetraazaanthracene derivatives have been considered theoretically to obtain information about their stabilities and aromaticities. The expected decrease of aromaticity of parent anthracene by tri or tetraaza substitution has been compensated by substitution of one of the hydrogens of the system by an electronegative group. The position of the substituent has been proved to be strongly effective on the aromaticity of the structure such that, the aromaticity is enhanced when the susbtituent is closer to the aza points.

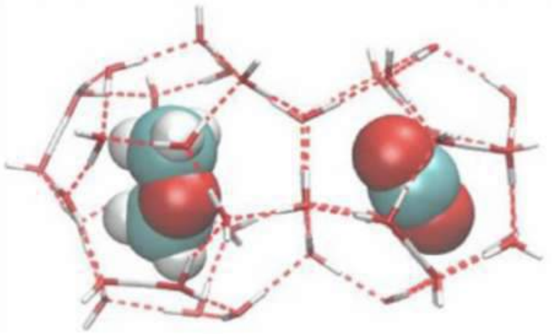
PP–49

Ab initio Studies on the SI Clathrate Hydrates

Zafer Maşlakcı[1], **Nevin Uras–Aytemiz**[2]

[1]Türkiye Bilim Evleri, Department of Chemistry, Isparta – Turkey
[2]Karabük University, Faculty of Science, Department of Chemistry, Karabuk – Turkey

Clathrate hydrates (called also as gas hydrates) are solid inclusion compounds consisting of an ice like network of host water molecules link through hydrogen bonding. Clathrate hydrates can be experimentally formed only in the presence of guest molecules. The guest-host interactions were studied with a model consisting of a combination of one small cage (5^{12}) and one large cage ($5^{12}6^{2}$). The small cage is filled with C_2H_2, CO_2, CH_4 and HCN guest gas molecules and large one is filled with simple ether molecules (i.e. DME, EO, TMO). The aim is to investigate the effect of small cage guest molecule on the large cage guest molecule stability. Calculations were conducted at M062X/cc-pvdz level. Host-guest interactions are examined by both atom-in-molecule and noncovalent interaction theories. This theoretical study supports the experimental studies of clathrate hydrates, which were prepared by different techniques and include different mechanisms of formation.



DME@$5^{12}6^{2}$+CO_2@5^{12}

ORGANIZERS

Nevin Aytemiz	Karabük University, Karabük – Turkey	nevinaytemiz@gmail.com
Murat Kılıç	EPFL, Lausanne – Switzerland	muratmkilic@gmail.com
Yavuz Dede	Gazi University, Ankara – Turkey	labydd@gmail.com

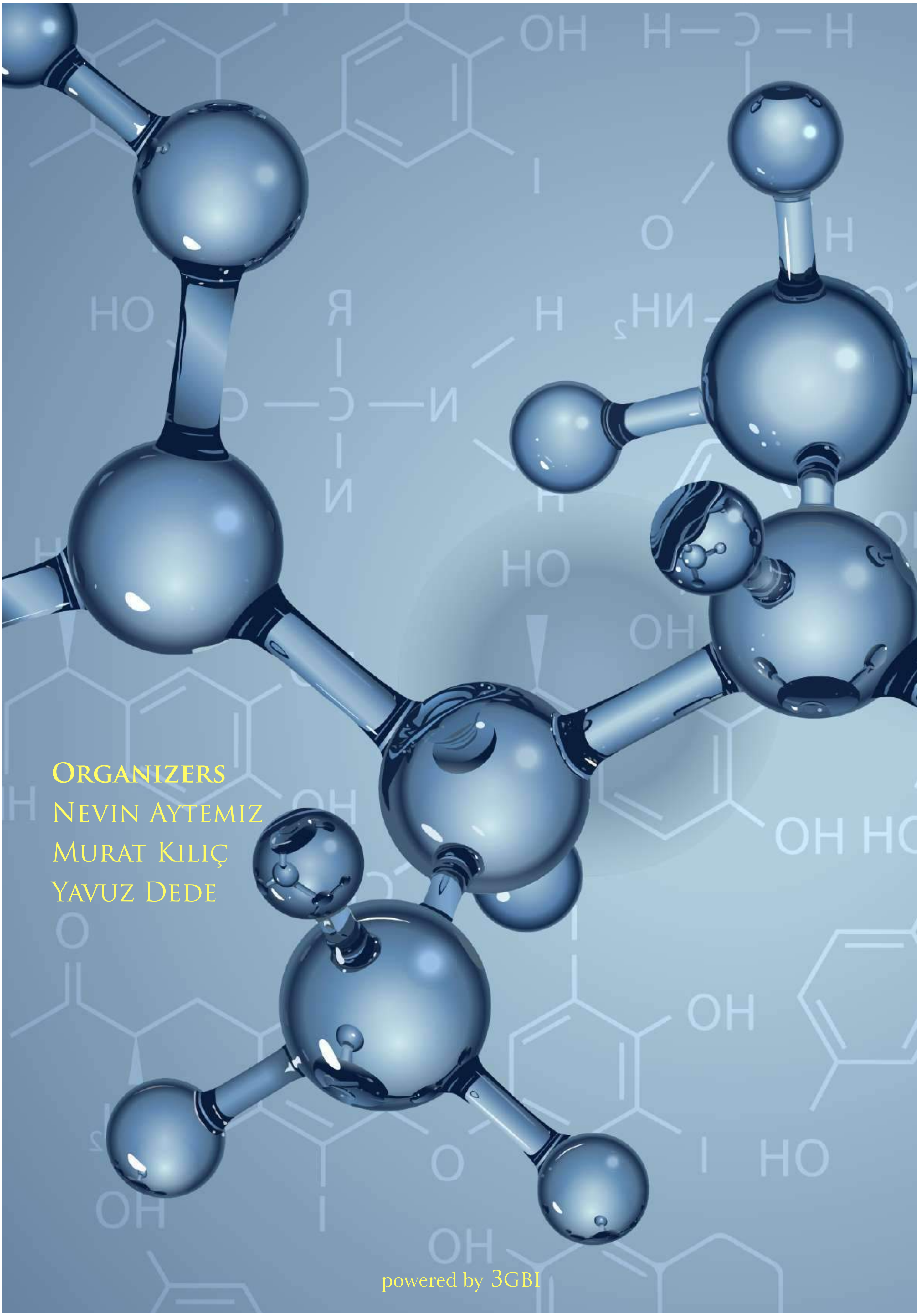
LIST OF PARTICIPANTS

(alphabetical order according to the last name)

1.	**Hande Abeş**	Yeditepe University , İstanbul – Turkey	handeabess@gmail.com
2.	**Nursel Acar Selçuki**	Ege University , İzmir – Turkey	nursel.acar@ege.edu.tr
3.	**Deniz Akgül**	Boğaziçi University , İstanbul – Turkey	denizakgul05@gmail.com
4.	**Sezen Alsancak**	Yeditepe University , İstanbul – Turkey	sezenalsancak@gmail.com
5.	**Cesur Altınkaya**	Yıldırım Beyazıt University , Ankara – Turkey	cesuraltnky@gmail.com
6.	**Kurt Arıcanlı**	Sabancı University , İstanbul – Turkey	aricanli@sabanciuniv.edu
7.	**Peter Armentrout**	University of Utah , Utah – United States	armentrout@chem.utah.edu
8.	**Evrim Arslan**	Boğaziçi University , İstanbul – Turkey	evrimarslan89@gmail.com
9.	**Nuran Asmafiliz**	Ankara University , Ankara – Turkey	gurun@science.Ankara.edu.tr
10.	**Şule Atahan – Evrenk**	TOBB University of Eco. & Tech., Ankara – Turkey	satahanevrenk@etu.edu.tr
11.	**Abdullah Atılgan**	Yıldırım Beyazıt University , Ankara – Turkey	bdllhtlgn@gmail.com
12.	**Canan Atılgan**	Sabancı University , İstanbul – Turkey	canan@sabanciuniv.edu
13.	**Öyküm Naz Avcı**	Boğaziçi University , İstanbul – Turkey	oykumavci@gmail.com
14.	**Viktorya Aviyente**	Boğaziçi University , İstanbul – Turkey	aviye@boun.edu.tr
15.	**Umut Aydemir**	Koç University , İstanbul – Turkey	uaydemir@ku.edu.tr
16.	**Şeyda Aydoğdu**	Yıldız Technical University , İstanbul – Turkey	aydogduseyda@gmail.com
17.	**Sefer Baday**	İstanbul Technical University , İstanbul – Turkey	badays@itu.edu.tr
18.	**Fatime Mine Balcı**	Süleyman Demirel University , Isparta – Turkey	minebalci@sdu.edu.tr
19.	**Bülent Balta**	İstanbul Technical University , İstanbul – Turkey	bbalta@itu.edu.tr
20.	**Turgut Baştuğ**	Hacettepe University , Ankara – Turkey	turgut.bastug@gmail.com
21.	**Esma Birsen Boydaş**	Ruhr-Universität Bochum , Bochum – Germany	esma.boydas@rub.de
22.	**Gülbahar Bozan**	İstanbul Technical University , İstanbul – Turkey	bozangulbahar@gmail.com
23.	**Uğur Bozkaya**	Hacettepe University , Ankara – Turkey	ugrbzky@gmail.com
24.	**Niyazi Bulut**	Fırat University , Elazığ – Turkey	bulut_niyazi@yahoo.com
25.	**Muhammed Büyüktemiz**	Gazi University , Ankara – Turkey	mbtemiz3@gmail.com
26.	**Yeşim Çamlısoy**	Yeditepe University , İstanbul – Turkey	ycamlisoy@gmail.com
27.	**Şaron Çatak**	Boğaziçi University , İstanbul – Turkey	saron.catak@boun.edu.tr
28.	**Murat Çavuş**	Bozok University , Yozgat – Turkey	murat.cavus@bozok.edu.tr
29.	**Nihan Çelebi Ölçüm**	Yeditepe University , İstanbul – Turkey	nihan.olcum@yeditepe.edu.tr
30.	**Zekiye Çınar**	Yıldız Technical University , İstanbul – Turkey	cinarz@gmail.com
31.	**Zehra Deniz Çırak**	İnönü University , Malatya – Turkey	deniz.cirak@inonu.edu.tr
32.	**Semih Danışmaz**	Bülent Ecevit University , Zonguldak – Turkey	semihdanismaz@hotmail.com
33.	**Naciye Durmuş İşleyen**	İstanbul Technical University , İstanbul – Turkey	durmusna@itu.edu.tr

34. **Sondan Durukanoğlu Feyiz** Kadir Has University , İstanbul – Turkey sondan@khas.edu.tr
35. **Derya Düzenli** Gen. Dir. of Mineral Research & Explorations , Ankara – Turkey duzenlid@gmail.com
36. **Özlen Ferruh Erdem** METU , Ankara – Turkey ozlenfy@gmail.com
37. **Volkan Fındık** Marmara University , İstanbul – Turkey volkan.findik@marmara.edu.tr
38. **Ali Emre Genç** Gazi University , Ankara – Turkey aegenc@gmail.com
39. **Sümeyye Gökce** TOBB University of Eco. & Tech., Ankara – Turkey zsumeyyegokce@gmail.com
40. **Tandaç Furkan Güçlü** Sabancı University , İstanbul – Turkey tguclu@sabanciuniv.edu
41. **Merve Güreşci** Ege University , İzmir – Turkey merveguresci@windowslive.com
42. **Emre Gürsoy** TOBB University of Eco. & Tech., Ankara – Turkey emre.grsy91@gmail.com
43. **Arzu Hatipoğlu** Yıldız Technical University , İstanbul – Turkey hatiparzu@yahoo.com
44. **Yusuf Serhat İş** İst. Gedik Uni. & İst. Technical Uni. , İstanbul – Turkey yusufserhatis@gmail.com
45. **Gökhan Kaçar** Trakya University , Edirne – Turkey gokhankacar@trakya.edu.tr
46. **Işık Kantarcıoğlu** Sabancı University , İstanbul – Turkey kantarcioglu@sabanciuniv.edu
47. **Nazan Kara** METU & Çankaya University , Ankara – Turkey nazAnkara0511@gmail.com
48. **Ferdi Karadaş** Bilkent University , Ankara – Turkey karadas@fen.bilkent.edu.tr
49. **Feyza Karasu Kılıç** Adolphe Merkle Institute , Fribourg – Switzerland feyzakarasu@yahoo.com
50. **Şeydanur Kaya** Kastamonu University , Kastamonu – Turkey seydanurkaya@kastamonu.edu.tr
51. **Hanifi Kebiroğlu** Fırat University , Elazığ – Turkey hanifi007@hotmail.com
52. **Seda Keskin Avcı** Koç University , İstanbul – Turkey skeskin@ku.edu.tr
53. **Armağan Kınal** Ege University , İzmir – Turkey armagan.kinal@ege.edu.tr
54. **Ali Can Kızılkaya** İzmir Institute of Technology , İzmir – Turkey alicankizilkaya@iyte.edu.tr
55. **Başak Koca** Boğaziçi University , İstanbul – Turkey basak.koca@boun.edu.tr
56. **Feyza Kolcu** Çanakkale Onsekiz Mart University , Çanakkale – Turkey feyzakolcu@comu.edu.tr
57. **Mediha Kök** Fırat University , Elazığ – Turkey msoglu@firat.edu.tr
58. **Oğuzhan Kucur** Boğaziçi University , İstanbul – Turkey oguzhan.kucur@boun.edu.tr
59. **Nermin Kutlu** Süleyman Demirel University , Isparta – Turkey kutlugulnermin@gmail.com
60. **Önder Küçükterzi** Ankara University , Ankara – Turkey onderkucukterzi@gmail.com
61. **Yves Leterrier** EPFL , Lausanne – Switzerland yves.leterrier@epfl.ch
62. **Zafer Maşlakcı** Türkiye Bilim Evleri , Isparta – Turkey zafermn@hotmail.com
63. **Hamissou Mohaman** Ondokuz Mayıs University , Samsun – Turkey mohamanhamissou.mh@gmail.com
64. **İpek Munar** Boğaziçi University , İstanbul – Turkey ipek.munar@boun.edu.tr
65. **Yıldız Ocak** Gazi University , Ankara – Turkey yldzocakk@gmail.com
66. **Cahit Örek** Kastamonu University , Kastamonu – Turkey cahitorek@gmail.com
67. **Ersin Emre Ören** TOBB University of Eco. & Tech., Ankara – Turkey eeoren@gmail.com
68. **M. Oluş Özbek** Yeditepe University , İstanbul – Turkey olus.ozbek@yeditepe.edu.tr
69. **Cem Özdoğan** Katip Çelebi University , İzmir – Turkey cozdogan11@gmail.com
70. **Emrah Özensoy** Bilkent University , Ankara – Turkey ozensoy@fen.bilkent.edu.tr
71. **Özge Özkılınç** Ankara University , Ankara – Turkey ozge_ozkilinc@hotmail.com
72. **Doğa Özşen** Yeditepe University , İstanbul – Turkey dogaozsen@gmail.com
73. **Işılay Öztürk** Ege University , İzmir – Turkey isilayozturk@gmail.com
74. **Osama Qandeel** Gazi University , Ankara – Turkey osamaqan@outlook.com
75. **Ulrike Salzner** Bilkent University , Ankara – Turkey salzner@fen.bilkent.edu.tr

76. **George Schatz** Northwestern University , Illinois – United States georgecschatz@gmail.com
77. **Helmut Schwarz** Technical University of Berlin , Berlin – Germany helmut.schwarz@tu-berlin.de
78. **Cenk Selçuki** Ege University , İzmir – Turkey cenk.selcuki@gmail.com
79. **Fethiye Aylin Sungur** İstanbul Technical University , İstanbul – Turkey aylin.sungur@itu.edu.tr
80. **Fidan Sümbül** Aix–Marseille Université , Marseille – France fidan.sumbul@inserm.fr
81. **Şefik Süzer** Bilkent University , Ankara – Turkey suzer@fen.bilkent.edu.tr
82. **Ufuk Şahin** Gazi University , Ankara – Turkey ufuksahinc@gmail.com
83. **Tuğçe Şener Raman** Ege University , İzmir – Turkey tgcsener@gmail.com
84. **Zeynep Turhan Irak** Iğdır University , Iğdır – Turkey zeynepsilanturhan@hotmail.com
85. **Yasemin Tümer** Karabük University , Karabük – Turkey yasemintumer@karabuk.edu.tr
86. **Nurcan Tüzün** İstanbul Technical University , İstanbul – Turkey nurcant@itu.edu.tr
87. **Pelin Ulukan** Boğaziçi University , İstanbul – Turkey pelin.ulukan@gmail.com
88. **Alper Uzun** Koç University , İstanbul – Turkey auzun@ku.edu.tr
89. **Aslı Ünal** Hacettepe University , Ankara – Turkey asliunal08@gmail.com
90. **Yelda Yalçın Gürkan** Namık Kemal University , Tekirdağ – Turkey yyalcin@nku.edu.tr
91. **Dilara Berna Yıldız** Gazi University , Ankara – Turkey dilarabernayildiz@gmail.com
92. **Mehmet Yıldız** Şeyh Edebali University , Bilecik – Turkey mhmtyldz07r@gmail.com
93. **Ersin Yurtsever** Koç University , İstanbul – Turkey eyurtsev@ku.edu.tr
94. **Mine Yurtsever** İstanbul Technical University , İstanbul – Turkey mine@itu.edu.tr



ORGANIZERS

NEVIN AYTEMIZ
MURAT KILIÇ
YAVUZ DEDE

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