BOOK OF ABSTRACTS

COST Training School

COST action CA21101 COSY

Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications

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Belgrade, 19th – 22nd September, 2023

The Training School of COST action CA21101 COSY

Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications

$19^{th} – 22^{nd}$ September 2023, Belgrade, Serbia

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by Ivana S. Đorđević & Dragan M. Popović

Welcome Message

We are pleased to welcome you all to the first Training School of the COST Action CA21101 - CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS (COSY).

The Training School "Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications" will cover the expertise in a broad field of multiscale modeling. The topics will include physical and chemical aspects of multiscale modeling of solids, gases, liquid mixtures, fluid-structure interaction and biopolymers (proteins and nucleic acids), focusing on a better understanding and recognition of issues relevant to the application of the novel computational approaches for modeling molecular systems either isolated or in confined environments, which may consist of enclosing molecular cages, surfaces, interfaces as well as of strong electromagnetic static or optical fields. Accurate characterization of phenomena of astrochemical relevance, using the most advanced spectroscopic techniques and the highest-level ab initio theories will also be included. The Training School will address modern problems where the system complexity involves multiple time scales. As a result, the scientific program is very broad. To achieve aims of the Training School we have a great team of eminent teachers from Spain, France, Switzerland, Italy, Sweden, Romania, Czech Republic and Serbia.

The scientific program consists of four days of lectures, complemented by exercises aimed to provide a practical insight into the selected problems from the different covered fields. We have also scheduled a poster session, where the trainees will have the opportunity to present their work, promote themselves and create new synergies with other attendees.

We are grateful to the sponsors, colleagues and friends for helping with the organization of this Training School. In particular, we are thankful to the COST Action CA21101 "COSY" for having provided the financial support, and especially to the COST Action Chair (Prof Maria Pilar de Lara-Castells) and Grant Holder (Prof Juan Carlos Hernandez-Garrido); the host institution (Institute for Chemistry, Technology and Metallurgy) in Belgrade, Serbia, for all the human, logistic, and complementary funding resources provided.

We would also like to express our gratitude to all of our teachers and all trainees for coming to this meeting and hope that you will have a very pleasant stay in Belgrade and plenty of interesting scientific discussions.

The Chairs of the 1st COSY Training School: Sonja Grubišić and Jiří Vaníček

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Energetics and Kinetics of Steps in Proton Pumping Mechanism of Mammalian Cytochrome *c* Oxidase

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Cytochrome *c* oxidase (CcO), the terminal enzyme of cell respiration, is responsible for processing most of the biological oxygen and generating electrochemical proton gradient in aerobic cells. The energy released from the reduction of molecular O_2 to H_2O is used to pump protons across the inner-mitochondrial membrane [1, 2]. Recent time-resolved optical and electrometric experiments on the O→E transition have anticipated a sequence of reaction steps for the proton translocation mechanism in CcO. Besides kinetic gating, the CcO pump function encompasses a mechanistic principle of conformational gating control that can help to prevent protons from backward outflow during the process. It was also found that Glu242, an essential residue in transferring pump protons to the proton-loading site (PLS) and chemical protons to the site of oxygen reduction, accomplishes the function of the gating site by avoiding simultaneous contact with the pump site, oxygen ligands in the BNC, and the proton-conducting D-channel. Moreover, the microscopic reversibility of the individual steps and the importance of kinetic barriers in maintaining the unidirectionality of the overall process in CcO is noteworthy [2, 3].

Here we have included the conformational gating by Glu242 into a framework of the proposed His291 pumping model [4]. DFT/electrostatic calculations are employed to obtain energetics of the proton and electron transfer reaction steps during the O→E transition [2, 3, 5–7]. In addition, transition state theory estimates activation energies and kinetic barriers from the rate constant of transitions. The energy profile of the reaction mechanism is studied by exploring how the redox state of the metal centers, dielectric solvation effects, and membrane potential gradient affect the energy levels and possible leakage of the protein pump through the Glu242 gating site. Particular emphasis is made on side reactions that may short-circuit the pump, resulting in a loss of proton pumping, and how this may be avoided in natural biological systems [2, 3]. CcO employs several control mechanisms and gating situations to ensure the proton translocation unidirectionality and prevent proton leak in the opposite direction.

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