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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IN SCIENCE AND TECHNOLOGY

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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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DFT/Solvation Continuum Electrostatic Calculations of Proton Pumping in Mammalian Cytochrome *c* Oxidase

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The intricate process of proton pumping in cytochrome c oxidase (CcO) is vital to cell respiration. By harnessing the power of oxygen reduction, CcO produces energy and pumps protons across the mitochondrial membrane, creating an electrochemical gradient. The coupling of protonation and redox reactions, as well as the electrostatic interactions between protonatable and redox-active groups, are pivotal in this process. Knowledge of the identity of proton-binding groups is paramount to interpreting the reaction mechanism in CcO, and protonation states of essential residues have been studied extensively by experimental and computational methods. Recent computational analyses have shed light on His291, a ligand of the Cu_B center, as a potential proton-loading site. With computer simulations that assess pK_as of critical residues, explore electron and proton pathways, and evaluate the energetics of PT and ET processes, we can provide a more in-depth understanding of the molecular mechanism and catalytic cycle of CcO. Combining the DFT electronic structure and energy calculations with reaction and protein field contributions allows self-consistent solvation energy calculations to be iteratively performed. Moreover, valuable insights into mechanistic details and energetics of proton pumping and coupled ET/PT reactions are gained at the atomic level [1–6]. With this knowledge in hand, we have the potential to discover innovative approaches for energy generation and propel the field of molecular pumps forward.

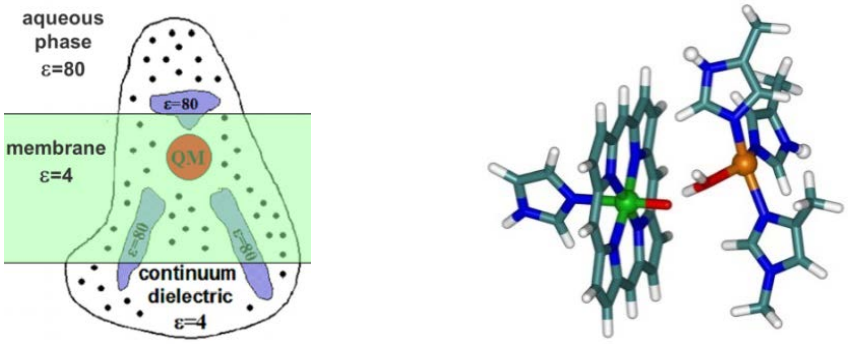

Fig 1. The DFT/SCE model of CcO with its quantum-mechanical part.

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