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EDITORIAL

International conference and workshop: Modeling and Design of Molecular Materials (10–15 September 2006, Wrocław, Poland)

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This special issue of the *Journal of Molecular Modeling* contains proceedings from a recent meeting held in Wrocław, Poland (http://www.mml.ch.pwr.wroc.pl/workshop/). This workshop continues the well-established tradition of previous Polish–Czech–American workshops in:

Nove Hrady in 2003 http://physics.mff.cuni.cz/kchfo/workshop03/, with proceedings published in the *International Journal of Molecular Science* [1],

Wrocław in 2004 http://www.mml.ch.pwr.wroc.pl/workshop/mdmm2004/, with proceedings published partly in the *Journal of Molecular Modeling* [2] with an extended form of some lectures also in a Springer book volume [3], and

Prague in 2005 http://physics.mff.cuni.cz/kchfo/workshop05/, with proceedings published in the *Journal of Molecular Modeling* [4].

The recent MDMM 2006 meeting in Wrocław was devoted to presentation of new developments in computational methods used in the modeling and design of new molecular materials and their applications. Experimental techniques (and their results) closely related to computational aspects were also presented during the workshop. In addition, Professors Lucyna Firlej (University of Montpellier II, France) and Bogdan Kuchta (University of Provence, France) conducted evening workshop tutorials—*Monte Carlo and statistics: modeling of molecular adsorption in nanoporous materials*.

This special issue contains 25 papers submitted by participants at the workshop, who presented 31 lectures and 57 posters in all.

First among the topics covered here is the theory of intermolecular interactions that constitutes the foundation of methods of rational design of molecular materials [3]. Application of various variants of density functional theory to the study of intermolecular interactions is discussed by Dułak and Wesołowski, whereas the work of Politzer et al. analyzes halogen bonding applications in crystal engineering. Szarek and Tachibana examine the field theoretical model of chemical interactions.

Ligand binding studies are covered in papers by Bryliński et al. and Grzywa et al., whereas Cundari et al. additionally examine the challenging issue of enantiomeric excess calculations.

Protein interactions are modeled in the paper by Kurciński and Koliński, and protein membrane channels for ions are discussed by Boiteux et al. Oxygen transport in human hemoglobin is studied by Orłowski and Nowak using locally enhanced molecular dynamics, whereas Pepłowski et al. analyze docking of various substrates in co-nitrile hydratase using molecular dynamics. Szyja and Brodzik use Grand Canonical Monte Carlo technique to model adsorption of aromatic hydrocarbons on SiO_2/TiO_2 catalysts. Marzec et al. investigate CCl_4 adsorption and phase transitions on graphite

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[5]—this paper was published in an earlier issue of the *Journal of Molecular Modeling*. Cysewski and Czeleń examine guanine oxidative damage in B-DNA telomeres. Wojdeł et al. model, via a periodic DFT approach, double metal cyanide catalyst. Grochala analyzes possible molecular environments facilitating reductive H_2 splitting.

Several papers are devoted to simulations of molecular properties. Jaroń et al. model the electronic structure of potential superconducting hydrides $Yb^{II}BeH_4$ and Cs_3-$Yb^{III}H_6$. Resonance Raman vibrational analysis of GFP chromophore by Andruniów and of simulated UV-VIS spectra of PMMA polymers with attached azobenzenes by Zaleśny et al. allow more detailed interpretation of the corresponding experimental results, whereas Niewodniczański and Bartkowiak study the hyperpolarizabilities of some betaine dyes. Cysewski examines acidities/basicities of 14 carboxylic acids and Chojnacki the proton transfer in periodic hydrogen bonded systems. Gorączko models the distribution of isotopomeric clusters of molecular ions.

Several related contributions deal with various chemical transformations. Alagona et al. model asymmetric catalysis in hydroformylation/cyclization processes. Dyguda et al. analyze the physical nature of the catalytic activity of ThiK kinase, finding dominant electrostatic effects. The oxidation mechanism of cytochrome P450 isoform CYP3A4 is presented by Shaikh et al. First principles molecular dynamics studies are applied by Machado et al. to explain passivation processes on metal surfaces.

The above papers serve to illustrate well not only the challenges in the field of molecular modeling techniques, but also the significant progress that has been achieved in the last few years towards solving practical problems in materials science and biotechnology. Once more we would like to express our gratitude to all workshop participants for their participation, valuable presentations and discussions, as well as to all authors for the contributions presented in this special issue. We hope to meet all of you again during the forthcoming meeting in Prague (8–13 September 2007 http://physics.mff.cuni.cz/kchfo/workshop07/).

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