Symposium 3: Computational Methods in Chemical Engineering: Physical Chemistry

Organizers:
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Abstract. The symposium focuses on the current state-of-the-art in "Computational Methods in Chemical Engineering: Physical Chemistry", as they lead to the next generation of methods, approaches, and research foci in the field. This field encompasses a broad range of problems and approaches: ranging from atomistic quantum mechanical calculation of molecules to computer aided modeling and simulation in the development, integration and optimization of industrial processes. Here we limit the symposium's thematic focus on topics that are under the general scope of "Physical Chemistry", in the broader sense, embracing traditional chemical engineering topics (e.g. thermodynamics, solutions, polymers) and looking forward to research directions where the field is expanding (e.g. life sciences, biological engineering).

Keywords: Computer Simulations; Molecular Modeling; Theory; Physical Chemistry; Chemical and Biological Engineering.
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SYMPOSIUM PREFACE

The symposium focuses on the current state-of-the-art in "Computational Methods in Chemical Engineering: Physical Chemistry", as they lead to the next generation of methods, approaches, and research foci in the field. Chemical Engineering, since its inception as a distinct discipline, has pioneered the efforts for the prediction of physicochemical properties of rather complex materials (molecular liquids, polymeric fluids, colloidal suspensions). From its engineering viewpoint it aimed at concrete results that could be, and have been, utilized for process control, design and optimization purposes. These efforts produced, and keep producing, fundamental advances in our understanding of "soft matter" and in our ability to model it. The Symposium aims at synthesizing methodologies (e.g., fundamental molecular models, empirical molecular models, simulations and simulation innovations, predictive use of basic findings) by bringing together researchers that have contributed to the various aspects of "molecular engineering".

In addition to contributed presentations, two invited keynote presentations are included in the symposium, by: **Alexei R. Khokhlov** (Moscow State University), on: "*Computer design of copolymers with desired functionalities*", and by **Arup K. Chakraborty** (Massachusetts Institute of Technology), on: "*How T-cells 'see' antigen: A crossroad of the physical, life and engineering sciences*". These invited overview talks are aimed not only to provide an in-depth presentation of the current state-of-the-art in Computer Modeling in the field, outlining the outstanding challenges and opportunities, and providing a vision for the future of the filed, but also to establish a framework for the rest of the symposium presentations, and bridge to the other symposia of the ICCMSE conference.

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THEMES AND PRESENTATIONS

Indicative of the themes, and also of the broad range of research efforts and scientific disciplines, covered under the auspices of Computational Methods in Chemical Engineering, even when focused on Physical Chemistry, is our partial[3] list of presentation in this symposium:

- (Invited, Keynote) Computer design of copolymers with desired functionalities, Alexei R. Khokhlov, *Department of Physics, Moscow State University, Moscow, Russia.*
- (Invited, Keynote) How T-cells 'see' antigen: A crossroad of the physical, life and engineering sciences, Arup K. Chakraborty, *Departments of Chemical Engineering, of Chemistry and of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA.*
- Conformational Properties Of Dendritic Homopolymers With Interacting Branching Points, P. Efthymiopoulos, M. Kosmas, *Chemistry Department, University of Ioannina, Greece.*
- Conformational Transitions of a Model Polymeric System near Attractive Surfaces: A Monte Carlo Study, A.N. Rissanou, S.H. Anastasiadis, I.A. Bitsanis, *Institute of Electronic Structure and Laser, Foundation for Research and Technology Hellas, Heraklion, Greece.*
- Equation-of-State model for temperature-responsive polymers with tunable response onset, E. Manias and A.M. Kisselev, *Departments of Materials Science & Engineering and of Physics, Penn State University, University Park, PA, USA.*
- Phase Equilibrium of Colloid Systems with Particle Size Dispersity: A Monte Carlo Study, M. Yiannourakou, I.A. Bitsanis, I.G. Economou, *Molecular Thermodynamics and Modeling of Materials Laboratory, Institute of Physical Chemistry, National Center for Scientific Research, "Demokritos", Aghia Paraskevi Athens, Greece, and Institute of Electronic Structure and Laser, Foundation for Research and Technology Hellas, Heraklion, Greece.*
- Modeling the Viscosity of Aluminosilicate Melts, S.A. Decterov, A.N. Grundy, I-H. Jung and A.D. Pelton, *Centre de Recherche en Calcul Thermochimique, Dèpartement de gènie chimique, Ècole Polytechnique de Montréal, Canada.*
- Molecular Modeling of Polydimethylsiloxane Mixtures, Z.A. Makrodimitri and I.G. Economou, *Molecular Thermodynamics and Modeling of Materials Laboratory, Institute of Physical Chemistry, National Center for Scientific Research "Demokritos", Aghia Paraskevi, Athens, Greece.*
- Odd Electrons Of Nanomaterials. A New Approach To Computational Chemical Engineering, E.F. Sheka, *Research Department, Peoples' Friendship University of the Russian Federation, Moscow, Russia.*
- Clustering of Proteins embedded in Lipid Bilayers: a Monte Carlo Study, M. Yiannourakou, L. Marsella, F. de Meyer, and B. Smit, *Centre Europeén de Calcul Atomique et Moleculaire, Lyon, France and Molecular Thermodynamics and Modeling of Materials Laboratory, Institute of Physical Chemistry, National Center for Scientific Research "Demokritos", Aghia Paraskevi, Athens, Greece.*
- Theoretical study of adsorption of star-polymers by mean field theory, G. Kritikos and A.F. Terzis, *Department of Physics School of Natural Sciences, University of Patras, Patras, Greece.*

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[3] Selected confirmed presentations at the time of this preface

Ioannis A. Bitsanis

Ioannis A. Bitsanis received a diploma in Chemical Engineering from the Aristotle University in Thessaloniki, Greece, and a Ph.D. in Chemical Engineering from the University of Minnesota, USA, from the department of Chemical Engineering and Materials Science. During 1988-89 he served as a Visiting Scientist at the IBM Almaden Research Center (San Jose CA), before joining as an Assistant Professor at the Dept. of Chemical Engineering of the University of Florida (Gainnesville, FL), where he was promoted to Associate Professor with tenure in 1996. In 1999 he joined FORTH-IESL as a Principal Researcher. His research involves atomistic and coarse grained simulations of nanoconfined liquids, organic-inorganic nanocomposites, polymer solutions, melts and solid polymer interfaces, complex polymeric sytems (stars, dendrimers, rodlike polymers), and colloidal suspensions (vitrification, crystallization).

Evangelos Manias

Evangelos (Vagelis) Manias received a B.S. in Physics from the Aristotle University in Thessaloniki, Greece, and a Ph.D. in Chemistry from U. of Groningen, the Netherlands. He subsequently carried out postdoctoral research in Cornell, before joining Penn State University in 1998, where he currently is an Associate Professor of Materials Science and Engineering and the Head of the Polymer Science and Engineering Program. His research combines simulation and experimental approaches focused on explaining how nanoscale structures affect the macroscopic materials properties in multi-phase polymer systems, and employing this fundamental understanding in the design of appropriate structures and functionalities that lead to high-performance novel materials and nanocomposites.