Foundations of Molecular Modeling and Simulation (FOMMS)

Foundations of Molecular Modeling and Simulation (FOMMS) is an international conference showcasing the applications and theory of computational quantum chemistry, molecular science, and engineering simulation. The motivation for this conference is the continual need for precise control of product properties, the accurate prediction of physical properties, and the development of a fundamental understanding of the chemical processes that allow the efficient creation of new products that meet specific marketplace demands. Theoretical and algorithmic advances along with modern computing technology routinely leads companies to capture the cash value of truly sustainable, far-reaching competitive advantage. A molecular-level understanding of these chemical processes lead to model mechanisms that are robust, pertinent, scalable, and most importantly, integratable across statistical, chemical, and engineering technologies. The future for these methods is extremely bright as they continue to prove their value to the chemical and chemical-related industries in the coming decade.

FOMMS 2009 is the 4th international conference, held every three years, in a distinguished series that focuses on the theory and practice of molecular modeling and simulation. The overall goal of the FOMMS conference series is to evaluate current progress in the molecular modeling and simulation field and to identify new intellectual challenges that may have a fundamental impact on future practice. The theme of the FOMMS 2009 conference, Foundations for Innovation, reflects recent advances and innovation in the fundamentals of molecular modeling and simulation and its application.

An important aim of FOMMS 2009 was to bring together and foster interactions among world-renowned experts from academia, government and industry, graduate students, and postdoctoral associates. Invited speakers discussed a broad range of theoretical and applied topics with applications in the chemical, petrochemical, pharmaceutical, materials, and energy related industries. Contributed posters allowed the presentation of recent research results and provided a forum for informal discussions. The first FOMMS medal was awarded to Professor Michele Parrinello for his contributions to the field of molecular simulation. A tutorial on graphics processors for scientific simulation and workshops on the development of open-source molecular simulation software and the use of simulation modules in education was held. Our hope is that the scientific contributions presented at FOMMS 2009 and included in these proceedings will stimulate new advances and innovations in molecular modeling and simulation.

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