Network for Computational Nanotechnology & c-PRIMED Seminar Series

Dr. Paul Saxe
President and CEO, Materials Design

Friday, October 16th at 3:30pm
Neil Armstrong Hall of Engineering, Room 1010

Atomistic Modeling: Past, Present, and Future, MGI, ICME, etc.

I will present a perspective on atomistic modeling — tools using quantum methods such as DFT, as well as molecular dynamics and Monte Carlo methods based on forcefields — over the past 30 years or so. While we are all caught up in the present, it is important to remember and realize how extraordinary the progress has been over time, both in the underlying computational power and in the methods and techniques. This then leads directly to what the future will look like, how these tools and others will fit into the framework envisaged by the Material Genome Initiative (MGI), ICME, etc. I have made my living selling this software commercially for the past 25 years, starting and running a company to enable this technology for industrial use, and so bring a different and hopefully useful perspective to the challenges ahead, both for atomistic modeling but also for MGI and ICME in the larger sense of their goal of transforming how industry approaches materials innovation.

Dr. Paul Saxe started his career in quantum chemistry, receiving his Ph.D. from UC Berkeley in 1982 under the guidance of Henry F "Fritz" Schaefer III. His work focused primarily on method development, pioneering some of the early implementations of e.g. SCF second derivatives and CI gradients. He continued this work at an NRC/NAS postdoctoral position with the Ballistics Research Lab (now the Army Research Lab) in Aberdeen, MD and then as a staff scientist at Los Alamos National Lab. In 1987 he moved to a startup company BioDesign, started by Prof Bill Goddard of Caltech, switching his focus to molecular dynamics for drug design, polymer as well as materials applications. In 1990 he moved to Biosym, managing all the computational codes which ranged from Discover, the leading commercial MD code, to quantum codes such as DMol and Turbomole. Biosym and BioDesign — now MSI — subsequently merged to for Accelrys which is now Biovia, a part of Dassault Systemes.

Dr. Saxe along with Drs. Erich Wimmer and John Harris left Biosym/MSI in 1998 to found Materials Design with the explicit goal of creating a complete suite of atomistic modeling tools for materials science and engineering. Materials Design has grown to 28 employees in the US and Europe. MedeA, which is a comprehensive environment for atomistic modeling, is used worldwide at about 400 sites, including about 100 industrial companies in areas ranging from energy — nuclear and oil & gas — automotive, aerospace, chemical and electronics industries, with applications to metallurgy, corrosion, catalysis, semiconductors, polymers, fluids, etc.

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