

CCP5 International Visitor Report

Dr. Glenn J. Martyna

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Talk

Simulating and modeling of materials with atomic detail at IBM: From biophysics to high-tech application.

The goal of simulation and modeling studies is to provide insight into important systems of scientific and technological interest. Today, approaching such problems involves treating accurately complex heterogeneous interfaces. The novel mathematical physics methods and parallel algorithms underlying the study of nanostructures are briefly given followed by applications to problems in engineering, physics, and biophysics. In particular, models of carbon-based transparent electrodes for use in thin film solar cells are described showing how expensive oxide materials effectively may be replaced. A new approach to DNA sequencing is discussed and a novel understanding of how the conformational properties of small fragments of the HIV glycoprotein gp41 are affected by each other and their environment is presented. Throughout the lecture, the importance of synergistic interactions between theory, simulation and experiment to generate new insights is stressed.

Programme

06/11/2011 arrival at Manchester International Airport.

07-08/11/2011 visiting University of Warwick (Coventry). Host: David Quigley at the Department of Physics and Centre for Scientific Computing (d.quigley @nospam@ warwick.ac.uk).

09/11/2011 visiting the Thomas Young Centre at Imperial College London. Host: Mike Finnis (m.finnis @nospam@ imperial.ac.uk).

10-11/11/2011 visiting University of Cambridge. Host: Robert Best (rbb24 @nospam@ cam.ac.uk).

12-15/11/2011 visiting University of Edinburgh. Host: Jason Crain (jason.crain @nospam@ npl.co.uk).

16/11/2011 visiting University of Sheffield (Department of Material Science and Engineering). Hosts: Frances Kirk (f.e.kirk @nospam@ sheffield.ac.uk) and Prof. John Harding (j.h.harding @nospam@ sheffield.ac.uk).

18/11/2011 visiting STFC Daresbury Laboratory. Host: Ilian Todorov (ilian.todorov @nospam@ stfc.ac.uk).

19/11/2011 departure from Manchester International Airport.

Resume

Dr. Glenn J. Martyna received his Ph.D. in Chemical Physics from the Columbia University and subsequently became a NSF Postdoctoral Fellow in Computational Science and Engineering at the University of Pennsylvania.

He was a tenured faculty member at Indiana University, Bloomington before joining IBM Research. In 2008, he was appointed an Honorary Professor of Physics at The University of Edinburgh, UK.

Dr. Martyna's research has focused on atomistic modeling of chemical, biological and materials processes, in particular, developing novel techniques that markedly increase the speed and efficiency of computer simulations and applying the methods to investigate important physical phenomena.

His recent biomedical work has centered on developing new DNA sequencing techniques and combining physical experiment and theory to impact therapeutic and anti-microbial peptide design and his work in materials science has led to a new low power, fast post-CMOS technology based on four Patents that is in development at IBM. Dr. Martyna has published over 100 peer reviewed articles, several of which have 500 or more citations.