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A Practical and Versatile Approach to Describe Quantum Effects in Complex Molecular Systems

Since Nature obeys quantum mechanics, nuclear quantum effects could play a non-negligible or even important role in chemical dynamics in many cases. The semiclassical initial value representation (SC-IVR) has been shown to be a promising way to describe quantum dynamical effects in condensed phases, with that all degrees of freedom are treated on the same footing. We will report our recent methodological progress in its linearized version (LSC-IVR) to make it a practical and versatile tool for complex/large molecular systems. Simulation results with comparison to experimental data will be demonstrated, from chemical reaction rates, transport properties to inelastic neutron scattering and infra-red (IR) spectroscopy etc.. An introduction will also be briefly mentioned on its implementation in the AMBER molecular simulation package.

Date: 09th April 2010 (Friday)  
Time: 11am – 12.30pm  
Venue: NTU SPMS CBC Building Level 2, Conference Room  
Host: Prof. Lee Soo-Ying

Biography of Dr. Liu Jian

Dr. Jian Liu received his B.S. in Polymer Science and Engineering from the University of Science and Technology of China and was awarded the highest prize (Guo Moruo Scholarship) for his academic performance.

Dr. Liu received his PhD from the University of Illinois at Urbana-Champaign under Professor Nancy Makri. The thesis title was "Quantum dynamics with classical and quantum trajectories".

After receiving his Ph.D. in Chemistry, he went to the University of California-Berkeley to undertake postdoctoral research with Professor William H. Miller. His work has focused on developing methodologies in semiclassical initial value representations (SC-IVR) that are practical for quantum dynamical simulations in general complex (large) molecular systems.