Interfaces on molecular scales

Steve Y.L. Tse

Department of Chemistry, The Chinese University of Hong Kong, Shatin, N. T. Hong Kong

stevetse@cuhk.edu.hk

Interfaces naturally arise in many areas of science and engineering. Since the 90s, there has been an increasing interest in understanding interfaces by computer molecular simulation because of at least two reasons. First, as computing power advances, the ability to model larger systems reduces the system size effects from the wall boundaries and allows accurate simulations of the interfaces. Second, there are simulation results that contradict well-known analytical results have since been confirmed by experiment. In this talk, I will briefly discuss some techniques and theory for studying the interfacial systems. Then, I will summarize our efforts for understanding the interfacial systems in the topics of ion/molecule propensity for air-liquid interfaces, coalescence of atmospheric aerosols, and dynamics of colloidal particles at liquid-liquid interfaces.