# “凝聚态物理-北京大学周二论坛”

**2007-10**

**时 间：** **2007 年 5 月 29 日（星期二）下午 15:00－16:40**

**地 点：** **北京大学物理大楼中 212 教室**

**报告题目：** **Predicting structures and properties of nano-materials**


**摘 要：** **Theoretical approaches have, in recent years, become indispensable tools for the prediction of structures and the determination of properties of nano-scale materials to complement experimental studies. In this talk, I will first give a brief outline of methodologies commonly used in these studies, including density functional theory (DFT)-based methods and semi-empirical approaches. I will then discuss a semi-empirical Hamiltonian developed by our group that is designed to circumvent the size-limitation associated with DFT-based methods on the one hand and to correct the non-transferability of conventional two-center semi-empirical Hamiltonians on the other hand. Specifically, this semi-empirical Hamiltonian includes the self-consistent (SC) determination of charge redistribution and environment-dependent (ED) multi-center interactions, two factors crucially important for the transferability of semi-empirical Hamiltonians. I will also discuss a quantum mechanics-based molecular dynamics (MD) scheme based on the SCED Hamiltonian and present an example of its application to predict the relative stability of silicon nanowires of realistic sizes with diameters up to 15 nm.**



**报告人：** **Professor Shi-Yu Wu, University of Louisville, U.S. A.**


**报告人简介：** **Professor S.Y. Wu received his Ph. D. from Cornell University and now leads a condensed matter theory research group at University of Louisville. The group currently has more than ten researchers and is generously supported by US federal agencies, including the NSF, DOE, etc.**

**研究方向：** **The study of complex systems with reduced symmetry, from the determination of their stable structures to the evaluation of their properties. Specifically, the major resources are currently placed on the study of Carbon- and Silicon-based nano- structures, including carbon nanotubes, carbon clusters, fullerenes, silicon clusters, silicon nanowires, and silicon carbide-based.**


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