## " 凝聚态物理-北京大学论坛 " 2008-06

时间: 2008年4月11日(星期五)下午15:00-16:40

地 点: 北京大学物理大楼中 212 教室

Density Functional Theory and its Applications

This talk starts with a review of the development of density functional theory (DFT). I then describe its implementation into state-of-the-art computations of complex processes in condensed matter physics and materials science. In particular I discuss how DFT can be used to study water, which is probably the most important and fascinating material in the world. Its structure, on surfaces and when confined in small spaces, is the crucial problem under this investigation. I believe a renewed interest in recent years on this topic due to great progress in DFT computations over the last decade. The presented results are for specific systems, but they are explained in simple physical pictures suggesting that they also hold for other cases.

报告人: 王恩哥院士

报告摘要:

王恩哥1990年获得北京大学物理系博士学位。1995年起任中国科学院物理所研究员。主要研究领域为薄膜/纳米结构生长机理,受限条件下水的报告人简介:形态,以及轻元素纳米材料的制备及物性分析。曾获世界华人物理学会"亚洲成就奖"(2003),德国洪堡基金会研究奖(2005),第三世界科学院物理奖(2005)。

联系教授: 吕劲副教授 电话:62756393, jinglu@pku.edu.cn