SEMINAR SERIES

北京大学工学院 材料科学与工程系

Multiscale Modeling of the Growth of Nanoparticles

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地　点：工学院 1 号楼 210 会议室

主持人：孙强 教授

内容简介：

Metallic nanoparticles, characterized by their size- and shape-dependent properties, are used in various applications including sensors, catalysis, plasmonics and electronics. Yet, their bulk production with well-defined morphologies is not well understood. Solution-phase polyol synthesis is the most popular method of production for nanoparticles in suspension. The key ingredient of this process is a polymeric capping agent that determines the relative growth rates of the nanoparticles' crystallographic facets. The capping mechanism depends on the nature of the structure-directing agent and its weight percentage with respect to the polyol. In this presentation, I will discuss how state-of-the-art atomistic modeling, based on *ab initio* and multiscale approaches may provide insights into the role of structure-directing agents. I will then discuss the growth of metal nanoparticles on two-dimensional supports and how metal-substrate interactions can dictate their growth modes.

报告人简介：

Dr. Saidi is a Professor in the Department of Mechanical Engineering and Materials Science at the University of Pittsburgh. He received a PhD degree in Physics from The Ohio State University in 2003. Dr. Saidi's research interests are focused on material's design using quantum mechanical and multiscale simulations. He is an expert in computational methods that span a wide range of accuracy levels and length scales, including force-fields, density-functional theory, quantum Monte Carlo and quantum chemistry methods. More recently, Dr. Saidi has used these tools to study advanced materials for energy-related applications in electrochemistry and photocatalysis, corrosion under extreme conditions, nanoparticle growth and morphology, ferroelectricity in oxides, and Raman spectroscopy.

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