学术报告

题　目　**Density-functional Embedding Theory: An Effective Way to Perform Multi-Scale Quantum Mechanics Simulations of Materials**

报告人　**Dr. Chen Huang （Florida State University）**

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地　点　**固体所新楼 520 会议室**

摘要： Accurate and detailed electronic structures are prerequisites for our understanding and prediction of the properties of materials. Ideally, one just needs to solve the Schroedinger equation which has been introduced for over 80 years. Unfortunately, the many-body nature of the Schroedinger equation makes itself extremely difficult to solve. Theories of varying levels of accuracy exist in the literature. Very accurate methods, such as the configuration interaction method, often have a prohibitive computational cost that scales exponentially with system sizes. Fast methods, such as the Kohn-Sham density functional theory, often have large errors that are difficult to determine and control. All these difficulties severely limit the predictive power of materials simulations. A promising way to overcome such obstacle is to perform quantum mechanics embedding simulations, in which the key region in materials is solved by highly accurate methods, with the unimportant regions to be solved by fast, physically correct methods. In this seminar, Dr. Huang will present their recent advances in quantum mechanics embedding theory. He will show how to perform quantum mechanics embedding simulations of materials in a seamless and first-principle manner. He will also discuss its application to resolving two long-term puzzles that are related to surface catalysis and metal corrosion: (a) the adsorption of carbon monoxide on copper surface; and (b) the counterintuitive oxidation process of aluminum surface.

Dr. Chen Huang is the assistant Professor in the Department of Scientific Computing at Florida State University. Before that, he worked as a postdoctoral research associate under the guidance of Dr. Arthur Voter and Dr. Danny Perez, in the Theoretical Division at Los Alamos National Laboratory. He received his Ph.D. in physics from Princeton University in 2011 under the guidance of Prof. Emily Carter. His research focuses on developing novel multi-scale methods to solve challenging electronic problems in materials. He has contributed significantly to the density-functional embedding theory. His work on embedding theory provides an effective and rigorous framework to perform multi-scale quantum mechanics simulations of heterogeneous materials. By using the embedding theory, he and coworkers have revealed the adsorption mechanism of carbon monooxide on copper surface, a critical step toward the understanding of methanol synthesis.

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