VIENNA COMPUTATIONAL MATERIALS LABORATORY

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TECHNISCHE UNIVERSITÄT WIEN Vienna University of Technology

Structural and Physical Properties of Atomic Clusters

A talk by Qinfang Zhang

Yancheng Institute of Technology

DATE / TIME: Monday, March 27th 2017, 4:00 p.m.

LOCATION: Erwin Schrödinger Lecture Hall, 5th floor, Boltzmanngasse 5, 1090 Vienna

Manipulation and deposition of gas phase clusters is of primary importance for the synthesis of nanostructured materials and for the development of industrial processes based on nanotechnology. By controlling the interparticle spacing and distribution pattern on nanometer scale, we can modify the electron transport properties of closely spaced nanoparticle array through the tuning of electron tunneling/hopping. Quantum-conductance-based hydrogen sensors consisting of films of closely spaced *Pd* clusters will be discussed in this talk. Furthermore, to understand the remarkable and unexpected physical properties of atomic clusters within a certain size range and temperature range, density functional theory calculation combined an empirical genetic algorithm (*GA*) simulation will be chosen to discuss the structural evolution of (*ZnO*)_n clusters and the possible magnetic switching on transition-metal doped *Si* Clusters.



