Structure, Dynamics and Thermodynamics of Nanostructures and Surfaces

Talat S. Rahman, Kansas State University

A microscopic, temperature dependent study of surfaces and nanostructures is invaluable as it provides information on the nature of the bonding between atoms in regions of low symmetry and coordination and gives insights into how the bonding and other characteristics vary with temperature. In this talk I will compare the energetics and vibrational dynamics of several flat, stepped, and kinked transition metal surfaces to examine the effects of variations in the local geometry and coordination on the local contributions to the free energy and to the relative stability of these structures. By extending the study to two-dimensional triangular islands on fcc(111) surfaces, and to single and multi-grained nanocrystals, I will show that unique features in the local vibrational density of states, which give rise to novel thermodynamic properties, can be traced to the changes in the force-fields between atoms in and near steps and kink-sites. In examining the relative stability of these structures, I will show that vibrational entropy makes an essential contribution. I will also present some recent results on the similarities and differences in the electronic structure of the two types of mono-atomic steps on vicinals of Cu(111).