School of Nano Science

School of PHYSICS

IPM Condensed Matter & Statistical Physics Group

Weekly Seminar

Heat Transfer and Diffusion, Quantum Energy Barrier of Vacancy in Metallic and Bimetallic Nanocluster

Invited Speaker:

Dr. Farid Taherkhani

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Abstract:

For the 55-atom of icosahedron (Ih) AuCu nanoclusters, the CTC as a function of temperature and copper doping exhibits a non monotonous peak at about 80% Cu molar content, with the CTC value for the pure copper nanoparticles in good agreement with the experiment. The CTC values for Au, Cu, and Au−Cu alloys in nanoform tend to be much lower than the corresponding values in bulk structures with heat transfer occurring also via a convection mechanism that is absent in the bulk. Heat transfer in bulk Au-Cu occurs with phonon mechanism.

Density-functional theory (DFT) result shows that effects of the simultaneous presence of a vacancy and Pt atoms are found to be simply additive when their distances are larger than first-neighbors, whereas when they can be stabilizing at low Pt content due to the release of strain by the Pt/vacancy interaction or destabilizing close to a perfect Pt(core)/Ag(shell) arrangement.

DFT result for truncated-octahedral (TO) silver nanocluster shows that minimum quantum energy barrier for vacancy in related to exchange of vacancy and silver in surface (100). Kinetic Monte Carlo algorithm result for site occupancies of TO silver nanocluster has the following order: surface (100)> core > surface (111). Kinetics Monte Carlo estimates 3 mille seconds for vacancy equilibration time.

Wednesday, 12 Khordad 95 (1 June, 2016), 2-3 pm

Farmaniyeh seminar room