Nanoalloys: playing fields of Alchemists revisited and refined

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Abstract:

In the quest for new materials not surprising alloying has been an age old recipe as depicted by the shiny colors of a goblet from the 4th century supposedly signifying the unique optical properties of bimetallic (Ag-Au) nanoparticles. Boom in the modern era of systematic investigations of the properties of materials at the nanoscale came with the finding in 1997 by Haruta of enhanced reactivity of Au nanoparticles. Striking catalytic, electronic, magnetic, vibrational, optical and mechanical properties of nanoparticles have since been reported. Bimetallic nanoparticles are even more intriguing as composition is yet another switch that may control its novel characteristics which are expected to be different those of the bulk alloy (for examples metals that do not mix in the bulk material are found to be miscible at the nanoscale). In this talk after a brief review, I will consider two types of nanoalloys: bimetallic nanoparticles and islets of one metal on facets of another. I will examine competing factors that may conspire to produce stable configurations in each case and track how the vibrational, chemical and electronic structural properties of these nanoalloys vary with size, composition, and local environment. In the case of the Ag-Cu nanoparticles, the focus will be on understanding the factors that control the relative stability of a set of 34-atom particles of varying composition and how vibrational properties may serve as signatures of alloy composition [1,2]. In the case of Pt islets on Ru nanoparticles, the focus will be on changes in electronic structural

properties induced by allowing that make this nanoalloy very attractive as a fuel cell anode catalyst [3]. References:

[1] M. Alcántara Ortigoza and T. S. Rahman, Phys. Rev. B 77, 195404 (2008)

[2] H. Yildirim, A. Kara, and T. S. Rahman, J. Phys. Cond. Matt. 21, 084220 (2009).

[3] S. Stolbov, M. Alcántara Ortigoza, T. S. Rahman, and R. Adžić, J. Chem. Phys.