

Substrate Adsorption on the Catalytic and Dynamic Properties of Metal Nanoclusters

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Metal nanoparticles are often dispersed in polymeric matrix or prepared in presence of other capping agents to prevent coalescence. Such stabilizers play a crucial role in determining the size and shape of nanoparticles. The first part of the seminar deals with the structural and energetic properties of polymer dispersed nanoparticles calculated using molecular dynamics simulations and density functional theory calculations. Atomistic details of interactions between polyvinyl pyrrolidone and few nanoparticle model systems, and their possible implications will be discussed. Free energy calculations unravel the mechanism by which the polymer matrix prevents flocculation. DNA–metal nanoparticle conjugates have been shown to exhibit unusual properties that are of great relevance in areas such as disease diagnosis and therapy, and fabrication of novel nano–electronic devices. In the second part of the talk, detailed density functional theory calculations on the binding modes and interactions between small gold clusters and nucleobases/DNA base pairs will be presented. Extensive analysis of various physicochemical properties of all the complexes reveal that combining structural modifications to DNA bases and binding to gold clusters can be effectively used to conceive molecular systems with desired optoelectronic properties. The effect of DNA base interactions with nanoclusters on the catalytic efficiency will be discussed by taking the prototypical CO oxidation reaction as an example. Tagging of the gold cluster with DNA bases significantly reduces the reaction barrier, and leads to a mechanistic crossover.

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PhD in computational chemistry, 2004. A postdoctoral fellowship in the University of Maryland Baltimore, 2004–2008. A faculty member in the International Institute of Information Technology in Hyderabad, India, since 2008. Currently, an Associate Professor and heads the Center for Computational Natural Sciences and Bioinformatics. His research interests are protein folding, transmembrane protein structure–property modeling, heterogenous nucleic acids, and nanocatalysis. He is a recipient of Young scientist medal from the Indian National Science Academy, Young Associate of the Indian Academy of Sciences, Innovative Young Biotechnologist award, and AICTE Career Award for Young Teachers. Recently he received the JSPS Invitation Fellowship, and was selected for the Distinguished Lecture Award by the Chemical Society of Japan. Author of about 80 papers in the areas of computational chemistry and biology.