CONTROL OF DIMENSIONALITY, STRUCTURE, AND REACTIVITY OF GOLD NANOCATALYSTS: 2-D OR NOT 2-D?

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Investigations of physical systems of small sizes and reduced dimensionalities, exhibiting discrete quantized energy level spectra and specific structures and morphologies, open avenues for systematic explorations of the physical factors that control the unique properties of nano-scale materials structures. Computationally-based theoretical modeling and simulations play an increasingly important role in modern materials science, chemistry, and biology, and they may be called "computational microscopies" [1]

In this talk we focus on factors that underlie and govern the emergent chemical catalytic activity of gold nanostructures [2]. Topics that will be discussed include [3]: (i) Structures of free and surface-supported gold clusters; (ii) Cluster-support interactions (anchoring) and the influence of surface defects; (iii) Electronic structure and charge-states of supported gold nanocatalysts, (iv) Water enhanced catalytic activity; ((v) Catalysis of CO oxidation by negatively charged gas-phase gold clusters (vi) Control of dimensionality, structure and reactivity of gold nanoclusters through metal-oxide support thickness and/or applied electric fields.

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