

Emergent materials phenomena in the non-scalable size regime

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Investigations of finite aggregates of small sizes and reduced dimensionalities open avenues for systematic explorations of the physical factors and unifying principles that underlie the transition from the atomic and molecular domain to the condensed phase regime. Such behavior, where the dependence of the properties of the system on its size does not scale with the system's physical size, but rather where *Small is Different* in an essential way, is emergent in nature; that is, the exhibited behavior is characteristic of the assembly of particles rather than being a property of the individual constituents, showing behavior on a larger scale than that characterizing the (relatively local) interactions between the elementary components of the system. Identification and understanding of the microscopic origins of such *emergent phenomena*, are of fundamental importance for elucidation of the principles of self-assembly and self-selection operative at the nano-scale, as well as of great potential relevance to technological developments at the dawn of the new millennium. These physical and methodological issues will be discussed and illustrated using results obtained through large-scale classical and quantum simulations.

Topics will include:

- (i) Formation mechanisms, mechanical, quantized electric conductance, and chemical properties of metal and semiconductor nanowires and their interconnections [1];
- (ii) Atomic-scale friction, control of friction through modifications of molecular architecture, and nanotribological processes in lubricated junctions [2];
- (iii) Generation, stability and breakup of nanojets [3a] and deposited fractal islands [3b];
- (iv) Nanocatalysis by small gold and palladium clusters [4], and guidelines for atomic-scale control of catalytic activity;
- (v) Spontaneous symmetry breaking leading to formation of crystallized clusters (Wigner electron molecules) in individual two-dimensional quantum dots, and quantum-dot-molecules [5],
- (vi) Emergence of magnetism in free and surface-supported small palladium clusters [6], and
- (vii) Charge transport in DNA [7].

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