# SMALL IS DIFFERENT: EMERGENT BEHAVIOR IN THE NANOSCALE

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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 and unifying principles that underlie the transition from the atomic and molecular domain to the condensed phase regime. Such behavior, where the properties do not scale with the reduced physical size, but rather where *Small is Different* in an essential way that can not be deduced through extrapolation from knowledge of bulk behavior, is *emergent* in nature. Often, the *new and different* behavior at the nanoscale can be traced to the circumstance where one (or more) of the physical dimensions of the material aggregate approaches a length-scale characteristic to a physical phenomenon (with different phenomena being characterized by different length-scales).

Gaining insights into the nature of physical and chemical systems of highly reduced sizes, and developing experimental and theoretical methodologies aimed at probing, manipulating and controlling them on the atomic and molecular level, are among the major challenges of current basic interdisciplinary research. Computationally-based theoretical modeling and simulations play an increasingly important role in modern condensed matter physics, chemistry, materials science, and biology. In particular, such studies, that may be called *"computational microscopies"*, allow explorations of complex phenomena with refined resolution in space and time [1].

The use of *atomistic simulations as tools of discovery* will be discussed and demonstrated through studies of: nanojets and fluid nano-junctions, hydrogen welding and switching in gold nanowires, the surprising nanocatalytic activity of small gold aggregates, post-ionization counterion-assisted hole transport in DNA and the mechanism of the reaction of ionized DNA with water that may cause mutagenesis and disease.

1. U. Landman, "Materials by Numbers: Computations as Tools of Discovery", perspective article in Proc. Nat. Acad. Sci. (USA) **102**, 6671 (2005).