Small is different: adventures and surprises in nanoscale computational microscopy

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Finite materials systems of reduced sizes exhibit discrete quantized energy level spectra and specific structures and morphologies, which are manifested in unique, nonscalable, size-dependent physical and chemical properties. Indeed, when the scale of materials structures is reduced to the nanoscale, emergent behavior often occurs, that is not commonly expected, or deduced, from knowledge learned at larger sizes. Characterization and understanding of the size-dependent evolution of the properties of materials aggregates are among the major challenges of modern materials science. Using computer-based first-principles quantum computations and simulations [1], often in conjunction with laboratory experiments, we highlight such behavior in diverse nanoscale systems, focusing on the following topics: (i) Self-assembly of free and supported metal nanocrystals with structure, stability, dynamics, mechanical response & nanocatalysis originating from superatom electronic shell-closure and atom packing [1, 2]; (ii) Electric-field-induced shape-transitions and electrocrystallization of liquid droplets [3]. (iii) Pathways of post-ionization proton-coupled-electron-transfer reactions in DNA, underlying mutagenesis and malignancy, and involving a segmented-water-wire transport mechanism [4]; (iv) Single and dielectron attachment, solvation, and hydrogen evolution in water clusters [5]; (v) Coexistence of correlated electron liquids and weakly-pinned Wigner crystals under magnetic fields in the fractional quantum Hall effect regime [6].

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