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Small is Different: 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 phenomena 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. Computer-based classical and quantum computations and simulations are tools of discovery of nanoscale emergent behavior [1]. We highlight such behavior in diverse systems, including: (i) Atomistic simulations of nanoscale liquid jets and bridges and the stochastic hydrodynamic description of their properties [2]; (ii) Metal nanoclusters and their self-assembled superlattices exhibiting stabilities and properties originating from superatom electronic shell-closing, atom packing, and interactions between protecting ligands [3]; (iii) Electric-field-induced shape-transitions and electrocrystallization of liquid droplets [4], and (iv) Symmetry-breaking and formation of highly-correlated Wigner molecules between electrons in 2D quantum dots and bosons in traps [5].

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