SMALL IS DIFFERENT: EMERGENT PARADIGMS AND ATOMICALLY PRECISE NANO STRUCTURES

Uzi Landman
School of Physics, Georgia Institute of Technology, Atlanta, GA 30332-0430

Finite materials systems of reduced sizes exhibit specific forms of aggregation, phases, structures and morphologies, quantized electronic shell structures, dimensionality cross-over, and size-dependent evolutionary patterns, which are manifested in unique, nonscalable, size-dependent physical and chemical properties. Indeed, when the dimensions of materials structures are reduced to the nanoscale, emergent phenomena often occurs, that are not commonly expected, or deduced, from knowledge gained at larger sizes. Discovery, characterization, understanding and possible utilization of such emergent behavior of materials in the nanoscale are among the major challenges of modern materials science. Progress in theses directions is greatly facilitated, or even predicated, by synthesis, fabrication, separation and measurements of atomically precise nanostructures, and by theoretical investigations of their unique structural, chemical and physical properties. Computer-based quantum computations, simulations and emulations, are tools of discovery which enable uncovering emergent behavior in the nanoscale [1]. In this talk we employ such simulations, often in conjunction with laboratory experiments, in explorations of several atomically precise nanostructures, to address some of the basic origins that underlie the unique behavior of size-selected materials in the nanoscale, and highlight computational microscopy investigations of nanoscale phenomena in diverse systems. These include: (i) Nanocatalysis by size-selected cluster catalysts of nanometer dimensions [2a] and reassessment of the specific activity and size sensitivity of heterogeneously catalyzed reactions, e.g. ethelene hydrogenation catalyzed by nano-size platinum clusters supported on magnesia or amorphous silica surfaces [2b]; (ii) Monolayer- protected metal nanoclusters [3] and their self-assembled superlattices [3b], exhibiting stabilities and properties originating from superatom electronic shell-closing, atom packing, and interactions between protecting ligands ; (iii) The electronic structure and electrical transport characteristics – manifesting Fabry-Pérot interference patterns, described with tight-bonding and a Dirac relativistic formulation with position-dependent mass terms – of graphene nanoribbons, GNRs, with atomically precise widths and edges, including segmented GNRs (characterized by width-dependent energy band-gaps) comprised of junctions between nanoribbons of varying width [4]; (vi) Symmetry-breaking and formation of highly-correlated Wigner molecules [5a] in electron quantum dots [5a] and ultracold fermionic atoms, e.g. a few 10^{-9}K ^{6}Li atoms in laser-generated double-well confinements [5b,5c], exhibiting antiferromagnetic ground states modeled with exact numerical solutions of the microscopic Hamiltonian and mapped onto Heisenberg spin-chain and cluster Hamiltonians, as well as the t-J model [5c], suggesting the employment of finite ultracold atom systems in fundamental studies of quantum magnetism and high-T_c superconductivity.

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