Structure, Dimensionality and Properties of Supported, Suspended and Interfacial Clusters

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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. Emergent physical and chemical phenomena at the nanoscale regime and the use of atomistic simulations as tools of discovery in this area [1] will be discussed and demonstrated through studies focusing on systems involving: (i) surface-supported nanoclusters, (ii) suspended clusters (in the form of interfacial nanowires), and (iii) quantum electron and boson clusters in 2D dots and cold-atom traps.

(i) Nanocatalysis by small gold clusters [2(a-c)]; Structure, dimensionality and chemical reactivity of surface-supported gold clusters; Control of the physical and chemical properties of supported clusters through the selection of support thickness [2(d, e)] and via the use of external electric fields [2(f)].

(ii) Nanowire formation mechanisms; Structural (atomic and electronic) properties, Mechanical response; Shuttling wire-suspended nanoclusters; Quantized electric conductance; Metal-insulator transition and local magnetic moments in oxygenated gold nanowires [1, 3].

(iii) Symmetry breaking phenomena resulting in formation of electron Wigner crystallites and rotating electron molecules in 2D quantum dots, and in the appearance of crystalline arrangements and rotating vortex clusters in atomic traps [4].

[1] U. Landman, Proc. Nat. Acad. Sci. (USA) 102, 6671 (2005).
[2] (a) U. Heiz and U. Landman, "Nanocatalysis" (Springer, New York, 2006); (b) U. Landman et. al.,"Factors in gold nanocatalysis: oxidation of CO in the non-scalable size regime", Topics in Catalysis 44, 145 (2007) ; (c) A. Sanchez et al., J. Phys. Chem. A 103, 9573 (1999); (d) D. Ricci et. al. Phys. Rev. Lett. 97, 36106 (2006); (e) C. Zhang, B. Yoon, and U. Landman, J. Am. Chem. Soc. 129, 2229 (2007); (f) B. Yoon and U. Landman, Phys. Rev. Lett., 100, 056102 (2008).
[3] U. Landman et al Science 248, 454 (1990); A. Marchenkov et. al., Phys. Rev. Lett. 98, 046802 (2007); Nature Nanotech. 2, 481 (2007); C. Zhang et.al. Phys. Rev. Lett., 100, 046801 (2008).
[4] C. Yannouleas and U. Landman, Rep. Prog. Phys. 70, 2067 (2007).