SMALL IS DIFFERENT: LARGE-SCALE SIMULATIONS FOR THE NANOSCALE

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When the spatial extent (size) of a material approaches a length-scale characteristic of a physical property or phenomenon, new and unique physical behavior emerges which can not be predicted through scaling or extrapolation from that in larger (bulk) sizes and for which small is different in an essential way**.** Such new behaviors, resulting from reduction to the nanometer-scale regime (accompanied often by cross-over between dimensionality classes), include spectral, transport, magnetic, optical, chemical and mechanical phenomena.

Several case studies of electronic structure investigations pertaining to the unique properties of nanoscale materials will be discussed. These include: formation mecahnisms and energetics, structures, mechanical properties and transport in metal nanowires and semiconductor wires connected to metal electrodes investigated via LSD calculations and ab-initio molecular dynamics simulations; first-principles investigations of size-dependent evolutionary patterns of the properties of clusters; heterogeneous catalysis by gold clusters supported on MgO (100); formation of electron-molecules (Wigner crystallites) in two-dimensional quantum dots.

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