SIZE, DIMENSIONALITY AND STRONG ELECTRON CORRELATION IN NANOSCIENCE

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Abstract

The quantum size effect and very strong electron correlation are two hallmarks of nano electronic structure. While the quantum size effect is a one electron property, electron correlation involves interactions among the electrons. In electronic structure theory, electron-electron repulsion causing correlation is normally considered only in an average (or mean field) sense, as for example in a single Hartree-Fock determinant. This is the simple molecular orbital model which is often a good approximation for molecules. In infinite systems this averaging treatment leads to delocalized electronic bands -- an excellent description of bulk 3D sp3 semiconductors. However in reality electrons try to instantaneously avoid each other; their relative motion is correlated. In nanoscience strong electron-electron repulsion and correlation create new collective states and cause new femtosecond kinetic processes. This is especially true in 1D and 2D systems. I discuss strong correlation in carbon nanotubes, graphene, zero dimensional quantum dots, , trans-polyacetylene chains, transition metal dichalcogenides, organic/inorganic Pb iodide perovskites, and pentacene van der Waals crystals. The independent contributions of screening and dimensionality are analyzed.

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