Max-Planck-Institut für Astrophysik
Garching, Germany
http://www.mpa-garching.mpg.de

Quantum Chemistry of Confined Systems

Tokuei Sako

sako@chem.s.u-tokyo.ac.jp

Department of Chemistry, School of Science, The University of Tokyo
Tokyo, Japan

and

Geerd HF Diercksen

ghd@MPA-Garching.MPG.de

http://www.MPA-Garching.MPG.DE/ opmolsrv/MolPhysGroup/

Max-Planck-Institut für Astrophysik
Garching, Germany

Advances in semiconductor technology during the last two decades has allowed to create very small spatial structures, so called quantum dots and wires, for which the quantum structure is resolvable. Quantum dots, also known as artificial atoms, may be modelled by confining electrons into an external potential. Similarly, foreign atoms and molecules embedded into liquid helium and helium droplets, into fullerenes and into zeolites may be modelled by confining atoms and molecules into an appropriate external potential.

Standard quantum-chemical models like the Hartree-Fock (HF) and the configuration interaction (CI) method have been applied to study the effects of spatial confinement of electrons, atoms and molecules. The confinement is modeled by an external one-particle anisotropic harmonic oscillator potential. The wavefunction is approximated by a linear combination of cartesian anisotropic gaussian functions. The calculations are performed using, among others, the OpenMol Program. In this contribution selected results of spectral properties, electron density distributions, and polarizabilities of confined electrons and atoms will be presented and analysed.