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Electronic states of confined 2-electron quantum systems

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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 harmonic oscillator potential. The wavefunction is approximated by a linear combination of gaussian functions. The calculations are performed using the OpenMol Program.

The spectral properties, the electron density distributions, the correlation energies, and the polarizabilities computed for the 2-electron quantum dot, for the Hydrogen anion and for the Helium atom in a sperical harmonic oscillator potential have been studied. The Hamiltonian, the basis sets and the quantum-chemical method used will be outlined. The results will be presented and discussed.