

I Motivation

For a realistic description of matter, description derived from first principle (so called ab-initio methods) which

missing

Since 1990, methods within the density functional formalism have been very successful across a number of disciplines in physics, chemistry and biology [1], as they enable calculations of the total energies, which in turn enable calculations of lattice dynamics, thermodynamical properties of matter or chemical reactions. These calculations are cheap in comparison to methods working with full wave functions, so that simple system can be run on a home computer today.