Density-functional theory : basic concepts, applications, strengths and weaknesses

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Over the past two decades density-functional theory (DFT) has become the most popular method used in the community of computational chemists and physicists for the investigation of molecules and solids properties. The rapidly growing usage of DFT is intimately linked to both the fundamental developments on exchange and correlation functionals and the increase of the computer power.

In this paper I will present some of the fundamental concepts of DFT. I will exemplified the successes of the method through a selection of results obtained in the realm of molecular (e.g. chemical reactivity, adsorption on surfaces, photoluminescent properties) and solid state (e.g. thermodynamics, mechanical and transport properties) applications. I will also underline the most common weaknesses encountered by the method but also the various ways of circumventing them.