Predicting electron correlation

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Density Functional Theory (DFT) is the most popular electronic-structure method dealing with the problem of electron correlation. An overview of the theory is presented including an assessment of its application to a variety of systems. Focus is given on its success to describe one-electron properties like the Fermi surfaces of metallic systems, but also on pathologic cases like the gaps of insulators and semiconductors.

An extension of DFT for the superconducting state (SCDFT) is also presented. SCDFT is a first principles theory, which can reproduce/predict superconducting properties like the transition temperature and the superconducting gap without any adjustable parameters. Present functionals can treat only phonon-driven superconductivity. The results of the application to elemental superconductors, MgB_2, and metals under pressure are in excellent agreement with experiment.

Finally, the Reduced Density Matrix Functional Theory (RDMFT) is reviewed. RDMFT is an alternative theory to DFT which deals also with the many-electron problem. We present a recipe for calculating the fundamental gap within RDMFT which gives results very close to experiment. We also present applications to molecular and solid-state systems. There are good reasons to believe that RDMFT is very promising for applications on systems that DFT results deviate from experiment.