A comparison of various new functionals describing the exchange-correlation interaction as applied to studies of graphene

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It was not too long ago that the terms “ab initio” and “first principles” were used to described modern electronic structure calculations since these methods were based on rigorous approximations to the quantum mechanics and entailed no experimental or semi-empirical fitting parameters. The landscape for these types of calculations has changed considerably over recent years where a range of different functionals have been constructed, where some of the essential ingredients are not quantum mechanical principles, but semi-empirical fitting to optimize results for particular types of problems, for example surfaces. In this paper, some of the new functionals for describing interactions between atoms such as semi-local functionals (LDA, AM05, PBEsol, PBE, rPBE), hybrid functionals (HSE06, PBE0, B3LYP), and screened exchange and Hartree-Fock will be applied to studies of graphene, which is chosen for some of its unique properties. In particular, adatoms involving hydrogen, lithium and beryllium on graphene and vacancies in graphene are studied for their energetics, equilibrium properties, band gaps (where applicable) and electronic structure.