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Semi-empirical density functionals

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Two aspects of the development of functionals for practical density functional theory calculations will be discussed. First I will report on the current status of range-separated functionals based on Becke's 1997 generalized gradient approximation, augmented with a range-separation that gives 100% exact exchange at long electron-electron distances. A family of 4 functionals, wB97, wB97X, wB97X-D and wB97X-2 have been developed based on physical arguments followed by parameter fitting with a diverse training set. Their performance is assessed on a yet-more diverse range of independent test data. The prospects for improving range-separated functionals by additional refinement of the form of the separator will be discussed and illustrated with comparative calculations. Second, if time and progress permit, I will discuss the development of functionals that correct a multi-configurational reference wave function, as opposed to the Kohn-Sham single configuration. In these cases, the reference system has partially interacting electrons, and the correlation functional provides the residual electron-electron interactions. An approach that naturally addresses the challenge of potentially double-counting electron interactions will be presented.