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Fast and accurate self-interaction-free methods for calculating electronic excitations MARTIN HEAD-GORDON, University of California, Berkeley — Time-dependent density functional theory methods achieve both success and disaster in describing electronic excitations in molecules. Most disasters, such as catastrophic failures for charge-transfer excitations, arise due to self-interaction errors. In this talk, I discuss recent progress on the development of self-interaction free methods for calculating electronic excitations. These methods are based on low-order many-body theory, using auxiliary basis expansions to obtain high computational efficiency. To obtain satisfactory accuracy from non-self-consistent treatment of electron correlations, the use of one or two empirical parameters is explored to scale same-spin and opposite-spin correlations. Using opposite-spin terms only yields a reliable and efficient method which is applicable to molecules in the 100 atom regime, with asymptotically fourth order scaling of computation with molecular size. While calibrated for good performance in the Franck-Condon region, the prospects for extension to conical intersections will be briefly mentioned.

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