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Towards accurate density-functional treatment of non-covalent interactions in complex systems

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Accurate treatment of intermolecular interactions is an outstanding challenge in density-functional theory. While numerous approaches are now capable of modeling small molecular dimers, it is unclear how applicable these methods are to larger systems. This talk systematically investigates errors in density-functional approximations for non-covalent interactions, applied to both dispersion-bound and hydrogen-bonded clusters. In particular, a combination of the large-gradient behaviour of the exchange functional and delocalization error, rather than three-body dispersion terms, are shown to determine the performance of a given method. Additionally, we attempt to develop an optimal range-separated hybrid functional to pair with the exchange-hole dipole (XDM) dispersion model for molecular clusters.