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The role of delocalization error in non-covalent interactions from dispersion-corrected density-functional theory ALBERTO OTERO DE LA ROZA, National Institute for Nanotechnology-NRC — Extensive benchmarking of dispersion-corrected density functional theory (dcDFT) methods has shown that it is nowadays feasible to calculate, with great accuracy, binding energies of small dimers and lattice energies of molecular crystals. However, there are many outstanding questions that can only be answered by a proper understanding of the interplay between base functional and dispersion correction. In this talk, I explore how delocalization error from the exchange-correlation functional impacts the calculation of non-covalent donor-acceptor interactions. Delocalization error arises from the failure of most functionals to model the long-range behavior of the exchange-correlation hole. Its primary consequence for non-covalent interactions is that the stability of donor-acceptor interactions is overestimated. Errors caused by delocalization error are particularly harmful in systems with strong and extensive hydrogen-bonded networks (water clusters and ice) or strong donor-acceptor interactions (halogen bonding), and can not be corrected using a pairwise dispersion correction. In addition, I present how delocalization error affects real-life applications of dcDFT, such as molecular adsorption on iron-oxide nanoparticles and surfaces.

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