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Application of the exchange-hole dipole moment dispersion model to surfaces and 2D materials (I)

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The exchange-hole dipole moment (XDM) method is a density-functional model of London dispersion based upon second-order perturbation theory. The XDM dispersion coefficients are non-empirical and depend directly on the electron density and related properties. XDM offers simultaneous high accuracy for a diverse range of systems due to the variation of the calculated atomic dispersion coefficients with the electronic environment. In this talk, we focus on applications of XDM to adsorption of small molecules and of graphene on noble metal surfaces. We also consider the interlayer interactions in 2D electrides, an unusual class of materials possessing interstitial electron layers sandwiched between cationic atomic layers of the solid.

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