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Determination of Surface-Substrate Adsorption Energy using the Exchange-Hole Dipole Moment MATTHEW CHRISTIAN, UC Merced, ALBERTO OTERO DE LA ROZA, NINT, ERIN JOHNSON, UC Merced — Calculated surface-substrate binding energies are usually underestimated because conventional density functionals do not include dispersion, which is necessary to capture the van der Waals interactions that lead to weak physiadsorption. The exchange-hole dipole moment (XDM) model is a non-empirical density-functional approach to model dispersion. Adsorption energies for several aromatic molecules and nuclebases on noble metal surfaces were calculated using B86bPBE-XDM. In this talk, I compare the calculated adsorption energies with experiment and present implications for future applications to modeling surface interactions.

[1] A. Otero-de-la-Roza and E. R. Johnson, *J. Chem. Phys.* **138** 204109 (2013).
[2] A. Otero-de-la-Roza and E. R. Johnson, *J. Chem. Phys.* **137** 054103 (2012).
[3] A. Otero-de-la-Roza and E. R. Johnson, *J. Chem. Phys.* **136** 204109 (2012).

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