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Understanding the role of London dispersion forces in molecular surface processes

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The interactions and dynamics of molecules at surfaces and within pores are essential to many chemical processes, ranging from molecular storage to catalysis and self-assembly. A molecular level understanding of molecule-surface interactions is crucial for tuning surface/pore selectivity and reactivity. While it is clear that strong chemisorption bonds facilitate these interactions, the role of weaker van der Waals (vdW) forces, which include London dispersion and π - π stacking interactions, are often unknown or overlooked. Recent advances in density functional theory (DFT) have now made it possible to reliably account for London dispersion interactions. In this paper, I will discuss the use of one such technique, the Rutgers-Chalmers vdW non-local correlation functional,^{1,2} to demonstrate how the inclusion of London dispersion forces is critical for a truly first principles understanding of processes sensitive to molecule-surface interactions, such as the loading of H₂ within porous materials and the chemisorption of organic molecules at surfaces. These works highlight the fundamental importance of London dispersion interactions in the broader context of chemical physics. This work was supported by the Department of Energy, BES, Materials Sciences and Engineering Division.³

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