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Benzene and pyridine on silicon (001) : a trial ground for long-range corrections in density functional theory OLIVER WARSCHKOW, JENNIFER BENNETT, The University of Sydney, JILL MIWA, Aarhus University, DAVID MCKENZIE, The University of Sydney, NIGEL MARKS, Curtin University
— The adsorption chemistry of benzene and pyridine on the silicon (001) surface is characterised by two prominent adsorbate configurations: a precursor structure bonded to a single Si-Si dimer and a tight-bridge configuration that bridges between two adjacent dimers. We examine here the performance of 20 density functionals to predict the relative stability of these two configurations. Disagreements between the predicted and experimentally observed preference point to the importance of long-range exact-exchange terms in these adsorbate systems. These corrections however tend to be detrimental to the prediction of adsorption and activation energies. We discuss this conundrum in terms of systematic exchange-correlation errors that scale with the number of molecule-surface bonds.

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