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Alkanes adsorbed on graphene: a vdW-DF study ELISA LONDERO, EMMA KARLSON, MARCUS LANDAHL, DIMITRI OSTROVSKII, JONATAN RYDBERG, ELSE-BETH SCHROEDER, Chalmers University of Technology — Studies of small chains of molecules adsorbed on graphene are important for application of graphene in possible devices, not least its use as a gas sensor for the detection of single molecules. In this work we present a density functional theory study of the first ten n-alkanes adsorbed on graphene using the vdW-DF functional. We compare our adsorption energies to temperature programmed desorption measurements finding a similar linear scaling with the number of carbon atoms in the chain. The presence of an offset when extrapolating to the case of no molecules on the surface is also confirmed.

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