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ABSTRACT

We present a literature collection of experimental adsorption energies over late transition metal surfaces for systems where we believe the energy measurements are particularly accurate, and the atomic-scale adsorption geometries are particularly well established. We propose that this could become useful for benchmarking theoretical methods for calculating adsorption processes. We compare the experimental results to six commonly used electron density functionals, including some (RPBE, BEEF-vdW) which were specifically developed to treat adsorption processes. The comparison shows that there is ample room for improvements in the theoretical descriptions.

KEYWORDS

Adsorption energies, benchmarking; adsorption; density functional theory; surface science; catalysis; van der Waals; transition metals; single crystal adsorption calorimetry; temperature programmed desorption