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A fully consistent spin formalism for the nonempirical van der Waals density functional vdW-DF[1] T. THONHAUSER, S. ZULUAGA, C. ARTER, Wake Forest University, K. BERLAND, University of Oslo, E. SCHRÖDER, P. HYLDGAARD, Chalmers University of Technology — We present a proper nonempirical spin-density formalism for the van der Waals density functional (vdW-DF) method. We show that this generalization, termed svdW-DF, is firmly rooted in the single-particle nature of exchange and we test it on a range of spin systems. We investigate in detail the role of spin in the van der Waals driven adsorption of H_2 and CO_2 in the linear magnets Mn-MOF74, Fe-MOF74, Co-MOF74, and Ni-MOF74. In all cases, we find that spin plays a significant role during the adsorption process despite the general weakness of the molecular-magnetic responses. The case of CO_2 adsorption in Ni-MOF74 is particularly interesting, as the inclusion of spin effects results in an increased attraction, opposite to what the diamagnetic nature of CO_2 would suggest. We explain this counter-intuitive result, tracking the behavior to a coincidental hybridization of the O p states with the Ni d states in the down-spin channel. More generally, by providing insight on van der Waals interactions in concert with spin effects, our nonempirical svdW-DF method opens the door for a deeper understanding of weak nonlocal magnetic interactions.

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T. Thonhauser
Wake Forest University

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