

Abstract Submitted
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A van der Waals density functional built upon the electron-gas foundation¹ PER HYLDGAARD, Chalmers Univ. of Technology, Dept. of Microtechnology and Nanoscience –MC2, KRISTIAN BERLAND, Univ. of Oslo, Dept. of Physics, SMN, ELSEBETH SCHRÖDER, Chalmers Univ. of Technology, Dept. of Microtechnology and Nanoscience –MC2 — The vdW-DF method is designed to be a systematic extension of the constraint-based generalized-gradient approximation (GGA) and can therefore serve as general purpose density functional [PRB 90, 075148 (2014)]. Yet the early versions can have issues both with bulk systems and with weak chemisorption. We present a recent nonempirical version, vdW-DF-cx [J. Chem. Phys. 140, 18A539 (2014), PRB 89, 035412 (2014)], that resolves these issues. The version is designed to have a consistent combination of exchange and correlation. We show that it performs well for inter-molecular binding and that it can even be better than PBE for describing cohesion and structure of molecules and solids. These results validate the robustness of the vdW-DF plasmon-pole model, which we show is closed linked to the exchange correlation hole of constraint-based GGA.

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