On the general-purpose nature of van der Waals density functionals

Per Hyldgaard¹

1) Chalmers University of Technology

Corresponding author: Per Hyldgaard (hyldgaar@chalmers.se)

An accurate account of truly nonlocal correlations is important for understanding, for example, van der Waals (vdW) binding among molecules, weak chemisorption of organics, cohesion in layered compounds and in bulk. It helps us predict material structure which in turn determines optical response and other functionality. The vdW density functional (vdW-DF) method starts from the electron-response description that underpins the generalized gradient approximation (GGA). It adds a systematic counting of zero-point energy shifts arising from the electrodynamical coupling of GGA-type exchange-correlation holes. My talk explains how this formal interpretation recently guided us to define a consistent-exchange vdW-DF version, termed vdW-DF-cx, and a proper spin vdW-DF formulation. The vdW-DF-cx seeks to link many-body physics input relevant for bulk matter with insight on the role of exchange in molecular interactions. The design is nonempirical and firmly rooted in the electron-gas tradition for crafting density functionals. My talk reports a broad testing, showing vdW-DF-cx is highly accurate in the description of many different types of systems. My talk also discusses the mechanisms that contribute to this good transferability of vdW-DF-cx and to the general-purpose nature of the vdW-DF method.