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Electron response in van der Waals density functionals

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There is significant interest in density functional theory (DFT) of dispersive or van der Waals (vdW) interactions and in DFT studies of sparse systems where vdW forces contribute to the cohesion and behavior. The Rutgers-Chalmers van der Waals density functional (vdW-DF) method [PRL **92**, 246401 (2004); PRB **76**, 125112 (2007)] is a nonempirical approach to calculate vdW bonding and for DFT characterizations of sparse matter. The vdW-DF framework is defined by a single exchange-correlation density functional that rests on a plasmon-type description for both semilocal components and for a parameter-free evaluation of nonlocal correlation. My talk summarizes a set of vdW-DF studies that seeks to map and analyze details in the vdW-DF electron-response nature. The purpose is in part to extract consequences that can facilitate an experiment-theory comparison that goes beyond binding geometries and energies. The aim is also to seek implications that can help develop the vdW-DF framework. I present an analysis of the relative importance of morphology, screening (image-plane formation), and collective effects in the vdW-DF description of molecular systems. In addition, I compare vdW-DF results with Cu(111) experiments that tests the electron-response behavior in terms of adsorption-induced band shifts, the form of the overall light-molecule physisorption potential, and the corrugation in the kinetic-energy repulsion of molecules at surfaces. Overall, the vdW-DF studies suggest the importance of benchmarking vdW methods across different length scales and by exploring the variation that arise when related structures have a different balance between exchange repulsion and vdW attraction.