Abstract Submitted
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Towards a more accurate van der Waals density functional IKUTARO HAMADA, National Institute for Materials Science — The van der Waals density functional (vdW-DF) of Dion *et al.* [1] has attracted considerable attention, because the functional is able to describe intra- and intermolecular bondings with different natures, e.g., covalent and van der Waals bondings in a seamless fashion within the framework of density functional theory. However, the accuracy of the functional is yet to be improved for the applications to various systems. Here I propose an exchange functional for the second version of vdW-DF [2], which improves the accuracy of vdW-DF. The keys in the improved exchange are the matching to the gradient expansion approximation in the slowly varying limit and the large density gradient behavior set in Becke's exchange (B86b)[3]. Systematic study on gas phase molecules, solids, and molecular adsorption demonstrates the applicability of the proposed functional to a wide variety of materials. [1] M. Dion *et al.*, Phys. Rev Lett. **92**, 246401 (2004). [2] K. Lee *et al.*, Phys. Rev. B **82**, 081101 (R) (2010). [3] A. D. Becke, J. Chem. Phys. **85**, 7184 (1986).

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