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Van der Waals density functional applied to adsorption systems[1]
IKUTARO HAMADA, Advanced Institute for Materials Research (AIMR), Tohoku University — The van der Waals density functional (vdW-DF) [1] is a promising density functional to describe the van der Waals forces within density functional theory. However, despite the recent efforts [2], there is still room for further improvement, especially for describing molecular adsorption on metal surfaces. I will show that by choosing appropriate exchange and nonlocal correlation functionals, it is possible to calculate geometries and electronic structures for adsorption systems accurately within the framework of vdW-DF. Applicability of the present approach will be illustrated with its applications to graphene/metal [3], fullerene/metal [4], and water/graphene interfaces [5].

[1] M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, B. I. Lundqvist, Phys. Rev. Lett. 92, 246401 (2004).
[2] See for e.g., K. Lee, É. D. Murray, L. Kong, B. I. Lundqvist, D. C. Langreth, Phys. Rev. B 82, 081101(R) (2010).
[3] I. Hamada and M. Otani, Phys. Rev. B 82, 153412 (2010).
[4] I. Hamada and M. Tsukada, Phys. Rev. B 83, 245437 (2011).
[5] I. Hamada (submitted).

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