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On the pseudopotential approximation in the van der Waals density functional calculations IKUTARO HAMADA, MARTIN CALLSEN, National Institute for Materials Science — The van der Waals density functional (vdW-DF)[1,2] is a density functional that is able to describe van der Waals and covalent interactions in a seamless fashion, and has been applied to a variety of systems. In practical calculations, the pseudopotential (PP) approximation has been employed, for which the PPs should be generated consistently for the chosen exchange correlation XC functional. However, usually PPs generated with a generalized gradient approximation (GGA) XC functional are used and the effect of the approximation to the XC functional applied in the PP generation is scarcely discussed. In this work, we discuss the appropriate XC functionals in the PP generation for the vdW-DF calculations. Furthermore, we compare the vdW-DF results for several systems using the PP's generated with appropriate XC and those with GGA XC[3].

[1] M. Dion *et al.* Phys. Rev. Lett. **92**, 246401 (2004).
[2] K. Berland, *et al.*, Rep. Prog. Phys. **78**, 066501 (2015).
[3] M. Callsen and I. Hamada, Phys. Rev. B **91**, 195103 (2015).

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