Abstract Submitted
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Van der Waals interactions based on maximally localized Wannier functions in ABINIT CAMILO ESPEJO, CINVESTAV-Unidad Querétaro, Universidad Jorge Tadeo Lozano, TONATIUH RANGEL, Université Catholique de Louvain, YANN POUILLON, Nano-Bio Spectroscopy Group - ETSF, ALDO ROMERO, CINVESTAV-Unidad Querétaro, XAVIER GONZE, Université Catholique de Louvain — We review the recent implementation[1] of the method to evaluate van der Waals (vdW) interactions based on maximally localized Wannier functions[2,3] in the DFT software ABINIT[4]. The implementation allows for the evaluation of vdW interaction energies for molecular and periodic systems on the same grounds and at a low additional computational cost as compared with a normal DFT calculation. Some results on test systems such as Ar_2, benzene dimer and graphene bilayer show both its reliabilty and performance. Discussion of new defined variables controlling the calculation and guide lines for the user will be presented along with an application to MoS_2 structure.

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