Van der Waals interactions in semiconductor solids GUO-XU
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The binding in semiconductor solids arises mainly from the covalent hybridization
of atomic orbitals. Hence, it is typically assumed that van der Waals (vdW) interac-
tions play a minor role for their cohesion. In order to probe this conventional wisdom
we develop a method to calculate accurate long-range vdW coefficients for ions and
atoms in crystals. We first assess the validity of the Clausius-Mossotti relation be-
tween the polarizability and dielectric function for bulk semiconductors by compar-
ing periodic TDDFT calculations to direct extrapolation of the frequency-dependent
TDDFT polarizability for finite clusters. We find a good agreement between these
two approaches for computing vdW $C_6(V)$ coefficients for a broad variation in the
unit cell volume V for diamond, Si, and Ge crystals. When using TDDFT@HSE
with the Nanoquanta kernel, the volume-dependent dielectric constant of Si and Ge
is in excellent agreement with experimental data. The crystal-field screening reduces
the vdW coefficients by a factor of two compared to corresponding free-atom and
effective hybridized $C_6[n(r)]$ values [1]. The use of accurate $C_6(V)$ coefficients in
the PBE+vdW method [1] improves cohesive properties of Si and Ge in comparison
to experimental data. [1] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**,
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