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Van der Waals forces in solids: Challenges for density functionals
GUO-XU ZHANG, ALEXANDRE TKATCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — While the importance of van der Waals (vdW) forces for binding between molecules is well established, their influence on the cohesive properties of solids remains to be quantified from first-principles. In particular, most state-of-the-art density functionals yield systematic deviations for the lattice constants, cohesive energies, bulk moduli and transition pressures for a range of solid-state systems. We evaluate the long-range C_6 dispersion coefficients for ions in solids and use them to assess the effect of the long-range vdW forces on the abovementioned cohesive properties of ionic (NaCl, AgCl, MgO) and semiconductor (Si, GaAs) solids. For all of these systems, we obtain consistently accurate results by coupling the long-range $C_6 R^{-6}$ dispersion energy with the Perdew-Burke-Ernzerhof functional for the short range. We compare our results for the cohesive properties with recently developed functionals for solids.

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