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Dynamical Screening of van der Waals interactions in nanostructures: Sublimation of fullerenes[1] ANDREW M. RAPPE, JIANMIN TAO, JING YANG, University of Pennsylvania — Sublimation energy is one of the most important properties of molecular crystals, but it is difficulty to study, because the attractive long-range van der Waals (vdW) interaction plays an important role. In this talk, I will discuss our recent work on the calculation of the sublimation of fullerenes, using efficient semilocal density functional theory (DFT), corrected with the dynamically screened vdW interaction (DFT+vdW), the Langreth-Lundqvist nonlocal vdW-DF, and the pairwise-based dispersion-corrected DFT-D2, to study the sublimation of fullerenes. We find that the short-range part, which accounts for the interaction due to the orbital overlap between fullerenes, is negligibly small. Our calculation shows that there exists a strong screening effect on the vdW interaction. On the other hand, higher-order contributions can be as important as the leading-order term. However, these two effects make opposite contributions, leading to significant error cancellation. We demonstrate that, by considering higher-order contributions and the dynamical screening, the DFT+vdW method can yield sublimation energies of fullerenes in good agreement with reference values, followed by vdW-DF and DFT-D2. The insights from this study are important for better understanding of the long-range nature

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