System-Specific Dispersion Damping for Enhanced Accuracy in DFT Calculations of Noncovalent Interactions

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Accurate modeling of non-covalent interactions is critical for understanding the structure and properties of molecular solids, liquids, and clusters. While dispersion corrections have significantly improved the reliability of density functional theory (DFT) for such systems, conventional approaches rely on fixed, empirically parameterized damping functions. Here, we show that dynamically optimizing these damping parameters for each system can yield near-exact agreement with high-level reference data. By tailoring the damping parameters on-the-fly, we can reduce the standard deviation of error distributions from roughly 1 kcal/mol to just 0.1 kcal/mol for benchmark sets such as S22 and S66. This system-specific optimization strategy not only boosts the accuracy but also enhances the transferability of dispersion corrections in DFT. These results bring DFT calculations closer to the precision of sophisticated wavefunction-based methods, all while retaining computational efficiency. In doing so, we highlight a promising new direction for the advancement of computational chemistry tools.