POSTER PRESENTATION

Toward Accurate van der Waals Modeling: A Comparative Study of Empirical and Physical Approaches Using *VMoPro* and *MoProViewer*

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Understanding molecular recognition, crystal packing, and biological processes including protein–ligand binding, protein folding, and macromolecular structure all depend on accurate modeling of non-covalent interactions. In this study, we introduce and evaluate two complementary van der Waals (vdW) models—empirical and physically grounded—for computing exchange-repulsion, dispersion, and total vdW interaction energies. A set of 21 atom-type-specific vdW parameters (σ, ε, δ, and γ) was derived via a least-squares optimization using the SciPy library and implemented in the *VMoPro* software. The empirical model yields highly accurate interaction energies, exhibiting a strong correlation (R = 0.990) with reference Symmetry-Adapted Perturbation Theory (SAPT) values from the extensive NENCI-2021 dataset[1] comprising 6,000 diverse molecular dimers. The physical model—implemented in *MoProViewer*[2]—utilizes electron density and transferred atomic polarizabilities[3] from the ELMAM2 database to estimate exchange-repulsion and dispersion energies[4]. The vdW energies determined using the physical model exhibit a significant correlation, R = 0.956, with SAPT data, and a distance-dependent analysis showed that correlation improves with increasing intermolecular separation (0.80 to 1.10 Å). Together, these results demonstrate that the empirical *VMoPro* model, supported by optimized parameters, offers a computationally efficient and accurate alternative to high-level quantum mechanical methods. The physical model further emphasizes the significance of accurate electron density and polarizability parameters are for correct vdW interaction estimation.

References

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