Public summary

Modeling intermolecular interactions is essential for understanding chemical and biological processes such as drug–receptor binding, protein folding, and the adsorption of molecules on surfaces. One of the most accurate and widely used methods for analyzing noncovalent interactions is Symmetry-Adapted Perturbation Theory (SAPT). This method not only computes the total interaction energy, but also decomposes it into contributions with clear physical meaning, providing insight into the nature of intermolecular forces.

One of these contributions is the so-called exchange energy – an effect that stems from the quantum nature of electrons. According to the principles of quantum mechanics, electrons are indistinguishable and cannot be definitively assigned to one of the interacting molecules. As the distance between molecules decreases, exchange effects become increasingly significant, and simplified models used to describe them lose accuracy. Current computationally efficient approximations assume that at most a single pair of electrons can tunnel between the molecules. While recent advances have allowed for exact treatment of tunneling effects, these approaches still neglect another crucial factor: the correlation of electron motion within each molecule.

The goal of this project is to develop a variant of SAPT without compromise – one that fully accounts for electron tunneling between molecules, while also incorporating the effects of intramolecular electron correlation. This will enable a rigorous investigation of how these two phenomena influence each other and will lead to more accurate modeling of intermolecular forces.