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Predictive Electronic Structure Methods for Model Charge Transfer Systems

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Ionization of non-covalent dimers (such as pi-stacked or hydrogen-bonded nucleobases) changes the bonding pattern from non-covalent to covalent, which induces significant structural and spectroscopic changes. The high density of states and open-shell character of the wave functions presents a challenge for ab initio methodology. Robust electronic structure methods will be discussed, and their relative strengths and weaknesses will be demonstrated by examples (water, benzene, uracil cations and their respective dimers).