Unconstrained by Reality: Adventures in Computational Physical Organic Chemistry

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One unique and deeply satisfying aspect of computational chemistry is the ability to learn about real molecular systems by studying fictitious ones. That is, unlike experimental chemists, computational chemists are unconstrained by reality. I will describe some of our efforts to understand non-covalent interactions involving aromatic rings, including π-stacking interactions and anion-π interactions. These interactions underlie myriad chemical phenomena, and understanding their origin is vital for everything from the rational design of organic electronic materials to drug design. We have gained a deep understanding of these interactions by asking simple questions and studying simple (and sometimes fictitious) molecular systems. The resulting physical models of these interactions turn out to be quite simple and intuitive, yet contradict deeply-held views in the chemical community.