New Mechanisms and Concepts for Organic Reactivity and Enantioselectivity From Computations

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The development of new asymmetric catalytic methods is experimentally challenging. It is also difficult to compute: multiple non-covalent interactions and solvation effects influence structures and stabilities. As a result, computational analyses have often lagged behind empirical studies. I will describe the result of collaborative studies in which mechanistic understanding and quantitative predictions derived from computation have led to new and improved experimental designs.[1] In particular, we have explored the mechanism and selectivity of several transformations proceeding via ion-pairing.[2] Computational studies have been used to design new catalyst structures which have been experimentally validated,[3] leading to new methods to control the reactivity and selectivity of ionic reagents in solution.[4,5]

References

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