How to Make an Enzyme: Computational Optimization of Electric Fields for Better Catalysis Design

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We consider natural and de novo enzyme design and factors such as active site energetics, entropy of individual residues, dynamical correlations of enzyme motions, and electric fields as a way to exploit the entire protein scaffold to improve upon the catalytic rate. Using these principles, we show how other biomimetic catalytic constructs can be formulated, illustrated by a supramolecular capsule gold catalyst for carbon-carbon reductive elimination.

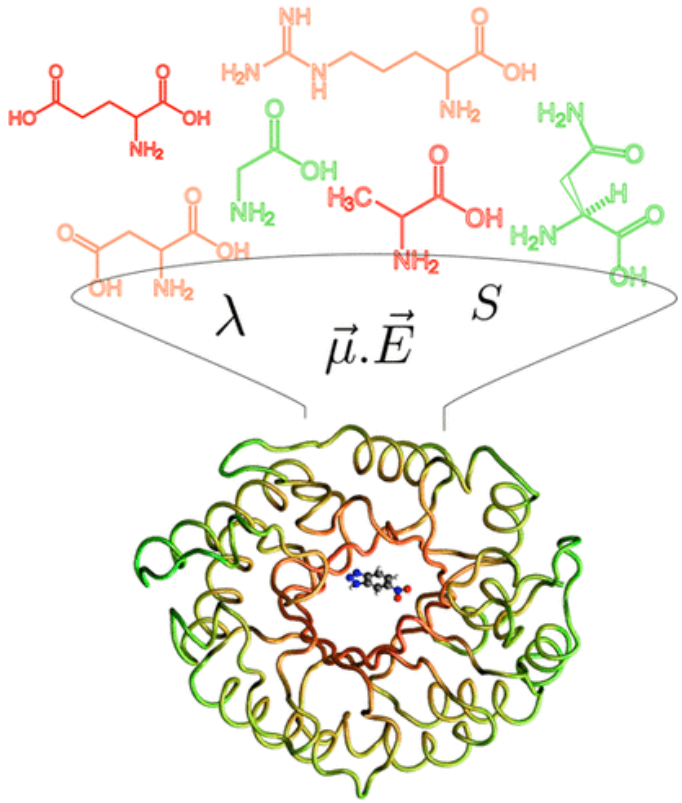

Figure 1: The origin of enzymes' remarkable performance has been the subject of extensive theoretical and computational research over the past several decades to design synthetic biocatalysts. This paves the way for building a unifying picture of the molecular interactions responsible for enzymes' incredible performance, hence managing efficient design and enabling further methods development for the accurate simulation of biomimetic catalysts.

References

1. V. Vaissier Welborn and T. Head-Gordon, *Chem. Rev.* (2018),in press link
2. V. Vaissier Welborn, L. Ruiz Pestana and T. Head-Gordon (2018), *Nature Catal.* 1, 649–655.