# Computational Modeling of Catalytic Reactions

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Computational modeling can provide insight into catalytic processes that augment experimental measurements. DFT calculations, combined with microkinetic modeling, provide detailed information on the elementary reaction steps. Combined with kinetic measurements, it allows the identification of side paths and alternative routes. Computational modification of the catalyst allows us to make predictions on improving catalytic performance. I will cover examples from metathesis [1], boron chemistry [2], and cooperative catalysis [3].

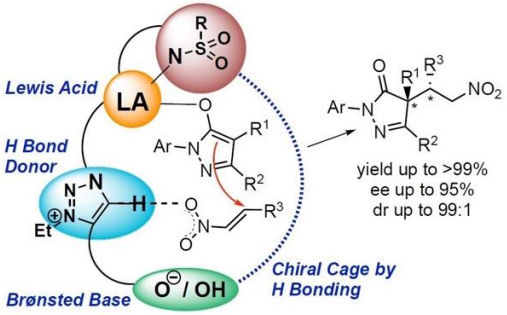


**Figure 1:** Active components in cooperative catalysis [3].

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