

Abstract Submitted  
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**Derivation and application of transition state force fields for enantioselective catalysis**<sup>1</sup> ERIC HANSEN, University of Notre Dame, PEROLA NORRBY, AstraZeneca, University of Notre Dame, University of Gothenburg, OLAF WIEST, University of Notre Dame — Standard methods of screening ligands for use in asymmetric, transition metal catalyzed reactions require experimentally screening hundreds of ligands, which is costly and requires specialized high-throughput machinery, and it is often a trial-and-error process. Accurate computational predictions of selectivity require extensive conformational sampling about the selectivity-determining transition state, but this process must be fast enough to compete with experimental screening techniques to be useful. Quantum to Molecular Mechanics can be used to computationally and rapidly predict the performance of ligands in asymmetric catalysis, while simultaneously providing an atomistic view of how they achieve their selectivity. The method has been applied successfully to a variety of transition metal catalyzed reactions that are both industrially and academically important. Herein, I will describe how we develop highly accurate molecular mechanics models of transition states from ab initio calculations and highlight several of their applications.

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