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Stochastic models form enhanced sampling in Chemistry

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The study of chemical reactions involving covalent links and breaks inherently presents stochastic complexities. To overcome the challenges posed by large energy barriers, researchers commonly use enhanced sampling techniques like transition path sampling and umbrella sampling to collect relevant data at the DFT level. However, the data acquired through these processes requires careful treatment to accurately infer any stochastic model. For transition path sampling, a realistic representation of the abort transitions is lacking, and for umbrella sampling, estimating the effect of external constant forces on the memory kernel is extremely challenging.

Within our team, we are developing innovative tools to address these issues. These tools aim to extract the true behavior of the reaction from the DFT data. The treatment of biases will then be employed to fit a quasi-Markovian Generalized Langevin Equation (GLE) model, enabling the extraction of meaningful insights beyond conventional DFT timescales.

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