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Huan Lei*, 2000 Stevens Dr, Apt 207, Richland, WA 99354, and **Nathan Baker** and **Xiantao Li**. *Quantifying quasi-equilibrium and non-equilibrium properties of biomolecule systems.*

Biomolecules exhibit conformation fluctuations near equilibrium states, inducing uncertainty in various biological properties near metastable states as well as transition between the states. We have developed a general method to quantify the uncertainty of target properties induced by conformation fluctuations. For local properties, to alleviate the high dimensionality of the conformation space, we propose a method to increase the sparsity by defining a set of collective variables within active subspace, which increases the accuracy of the surrogate model. For dynamic properties, we develop a data-driven method to evaluate the memory kernel of the energy-dissipation process based generalized Langevin Equation. The method is demonstrated on solvation properties and is generalizable to investigate uncertainty in numerous biomolecular properties. (Received September 15, 2016)