Finding Free Energy Landmarks of Reactions in Solutions

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We propose a novel approach to search for free-energy landmarks[1], i.e., minima and the saddle points, of chemical reactions in an automated manner using a combination of steepest descent and gentlest ascent methods. This technique opens a way to identify free-energy landmarks of bond-breaking/creating processes in which the underlying potential energy surface is described using on-the-fly electronic structure calculations. As demonstrations of the approach, we present an example of SN2 reaction in aqueous solutions using QM/MM simulations.

[1] M. Shiga, M.E. Tuckerman, *J. Phys. Chem. Lett.*, **2018**, *9*, 6207-6214