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agnostic machine learning description of chemical reactions in solution

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We address the problem of the training of a machine learning potential (MLP) for the atomistic study of rare events. By training a MLP only on a few dozens of agnostic out of equilibrium *ab initio* trajectories shot from the top of the barrier, we are able to recover free energies close to *ab initio* accuracy. As well as showing that it is possible to recover transition rates and transmission coefficients using the reactive flux formalism. Contrary to previous works, this training process does not need the prior knowledge of the detailed reaction mechanism. This method allows to study chemical reactions in solution with explicit solvent with a lesser computational cost. To do so we use the deepmd package on a widely studied reaction which is the SN2 substitution of methyl chloride.

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