Free energy reconstruction from steered dynamics: applications to vacancy migration in Fe, phase coexistence in FeCr and structural transitions in LJ38 MANUEL ATHENES, CEN Saclay, MIHAI-COSMIN MARINICA, SRMP CEA Saclay, GILLES ADJANOR, MMC, EDF Centre des Renardieres — Various methods achieving importance sampling in ensembles of nonequilibrium trajectories enable to estimate free energy differences and, by maximum-likelihood post-processing, to reconstruct free energy landscapes. Here, based on Bayes theorem, we propose a more direct method in which a posterior likelihood function is used both to construct the steered dynamics and to infer the contribution to equilibrium of all the sampled states. The method is implemented with two steering schedules. First, using non-autonomous steering, we calculate the migration barrier of the vacancy in Fe-α and the solubility of Cr in Fe-α. Secondly, using an autonomous scheduling inspired by metadynamics, we accurately reconstruct the two-dimensional free energy landscape of the 38-atom Lennard-Jones cluster as a function of an orientational bond-order parameter and energy, down to the solid-solid structural transition temperature of the cluster and without maximum-likelihood post-processing.

Manuel Athenes
CEN Saclay

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