Off-lattice kMC simulation of Pt alloy nanoparticle degradation

This study focuses on understanding the degradation mechanisms of Pt_3Co nanoparticles, which are crucial for fuel cell catalysts. We develop a machine-learned potential (MLP) for simulating the degradation processes, comparing its accuracy to density functional theory calculations. Utilizing off-lattice kinetic Monte Carlo simulations with the MLP, we replicate experimental trends and offer insights into atomic orderings. The findings suggest design principles for high-activity, durable Pt_3Co nanoparticles and validate the method's applicability to other alloy systems like Pt_3Ni and $Pt_3Co_{0.5}Ni_{0.5}$. This research provides a guideline for developing MLPs for alloy electrochemical catalysts and contributes to the design of more effective fuel-cell catalysts. This work was published at ACS Catalysis 2023, 13, 16073.