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**Using Cluster Expansions to Model Diffusion in Pt-Ni Nanoparticles** THOMAS NILSON, TIM MUELLER, LIANG CAO, Johns Hopkins Univ — Pt-Ni alloys have been shown to have excellent catalytic activity for the oxygen reduction reaction. However in practice these particles suffer from Ni dissolution, degrading the performance of the catalyst over time. The exact mechanism by which this occurs is unknown and difficult to determine experimentally. Using density functional theory, we have calculated the energies of formation of several dozen PtxNix-1 nanoparticles with included vacancies and used this data to parametrize a cluster expansion. Because the activation energies for diffusion are included in the model, we are able to use the cluster expansion to rapidly predict the transition rates in a Pt-Ni nanoparticle as a function of particle shape, size, and local atomic order. By using the cluster expansion model in a kinetic Monte Carlo algorithm we are able to model the diffusion of Pt and Ni and provide insights into the dissolution of Ni from Pt-Ni nanoparticles.

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