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Ab initio thermodynamics and kinetics for coalescence on nanoislands and nanopits on metal(100) surfaces[1] JIM EVANS, YONG HAN, Iowa State Univ, CONRAD STOLDT, University of Colorado, PATRICIA THIEL, Iowa State Univ — Coalescence or sintering of nanoscale features on metal(100) surfaces is mediated by periphery or edge diffusion. These processes are highly sensitive to the multiple diffusion barriers for various local edge environments. We provide an optimal strategy to determine both thermodynamics and kinetics for these systems at the ab initio level. The former requires assessing conventional interactions between adatoms at adsorption sites. The latter requires assessing unconventional interactions between the hopping atom at a bridge site transition state and other nearby atoms. KMC simulation reveals that this formulation recovers observed sintering times for Ag nanoislands on Ag(100), including a novel size dependence. The formulation also applies for nanopits where there are additional challenges to capture kinetics. See J. Phys. Chem. C 120 (2016) 21617.

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