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Nucleation pathways in partially disordered lattice models DAVID QUIGLEY, YURI LIFANOV, BART VORSELAARS, University of Warwick — Simple lattice models are attractive for the study of non-classical nucleation and growth from solution, a phenomenon still largely inaccessible to atomistic simulation. We have extended the Potts Lattice Gas (PLG) model of Duff and Peters to include a metastable partially ordered precursor phase, mimicking the common mineral calcium carbonate. Using a combination of multicanonical Monte Carlo and equilibrium path sampling, we demonstrate that thermodynamically favourable pathways between a metastable solution state and the fully ordered lattice proceed via formation of partially ordered nuclei. By comparing the activation energy associated with the ordering of these nuclei to that needed to nucleate the ordered phase directly, we demonstrate dissolution and re-precipitation as an emergent growth phenomenon of our model.

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