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Coarse Molecular Dynamics Applied to the Study of Structural Transitions in Condensed Matter MIGUEL A. AMAT, Department of Chemical Engineering, University of Massachusetts, Amherst, MA, IOANNIS G. KEVREKIDIS, Department of Chemical Engineering, Princeton University, Princeton, NJ, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, Amherst, MA — We report results from application of two coarse molecular-dynamics (MD) methods to determining the onset of structural transitions in condensed matter focusing on the melting of crystalline silicon. The two techniques require properly defined coarse variables that are slow and attracting. The first method is coarse projective integration. It allows wrapping a coarse time stepper around an MD simulator to extract the corresponding *coarse*-level description resulting from short MD bursts, which is used to extrapolate forward over coarse time steps. The second method is used to construct the underlying effective free energy landscape. Proper multi-system initialization at representative points in coarse-variable space along with analysis of the coarse-variable trajectories yields the effective free energy landscape upon integration of the reconstructed Fokker-Planck equation. Subsequent application of a coexistence criterion yields the thermodynamic melting point.

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