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Solidifying semiconductor nanocrystals from melts: Molecular dynamics simulations TIANSHU LI, DAVIDE DONADIO, GIULIA GALLI, Department of Chemistry, University of California, Davis — Understanding the nucleation of semiconductor nanocrystals is of fundamental importance in the field of nanoscience. In this study we employ classical molecular dynamics simulations to explore the crystallization of Si nanocrystals from the melt. We focus on the differences between homogeneous and heterogeneous nucleations, where the heterogeneous case is investigated by simulating a liquid slab. In particular, we use the recently developed forward fluxing method [R.J. Allen, D. Frenkel, and P.R. ten Wolde, JCP 124 024102(2006)] to model the evolution of nucleation processes from melts and to compute nucleation rates. We demonstrate that free surfaces act as catalytic nucleation sites by significantly promoting the formation of solid-like small clusters. The presence of solid-like clusters in proximity of the surfaces is found to occur at temperature higher than those at which solid seed nucleation occurs in bulk liquids, highlighting the important role of heterogeneous nucleation under low under-cooling conditions.

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