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Thermodynamics and kinetics of group-IV nanoparticles under pressure MATTEO COCOCCIONI, DMSE and ISN Massachusetts Institute of Technology, FRANCESCO MAURI, LMCP Universite' Pierre et Marie Curie, Paris, GERBRAND CEDER, NICOLA MARZARI, DMSE and ISN Massachusetts Institute of Technology — The kinetics and thermodynamics of phase transformations in group-IV nanoparticles during a shock compression are studied with full first-principles molecular dynamics simulations. A novel electronic-enthalpy functional is introduced to describe accurately and efficiently finite-size quantum systems under pressure. Significant differences are found in the structural response of carbon, silicon and germanium nanoparticles, depending on size, composition, and surface structure. The presence of trapped metastable amorphous configurations for Si and bigger Ge nanoparticles highlights the importance of kinetics effects in the phase transformation. It also demonstrates the possibility of using nanoparticles to study bonding rearrangements and structural transformations which are not accessible to the bulk counterparts.

Matteo Cococcioni
DMSE and ISN Massachusetts Institute of Technology

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