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Pressure-induced structural transformations in nanomaterials: a linear-scaling DFT investigation[1] NICCOLO CORSINI, PETER HAYNES, Imperial College London, CARLA MOLTENI, Kings College London, NICHOLAS HINE, Cambridge University, CDT TSM COLLABORATION — Semiconductor nanomaterials display a number of peculiar and tunable properties that distinguish them from their bulk counterparts. Of particular interest is their response to applied pressure, as they transform from one crystalline or amorphous structure to another. Accurate simulations are important for understanding finite size effects in the atomistic mechanisms of phase transformations (difficult to observe clearly in macroscopic experiments), for the opportunity to uncover novel metastable phases stabilized in finite systems, and for potentially innovative applications of nanomaterials. First-principles methods are essential to accurately describe the bond breaking/making in phase transformations and the realistic description of surfaces (often covered by complex surfactants). However the computational cost limits both the length- and time-scales attainable. We have combined an O(N) density functional theory code for large systems and an electronic-enthalpy method[1] to apply pressure to finite systems to model with quantum mechanical precision processes induced by pressure in nanomaterials under realistic conditions. The focus is on Si, Ge and CdS nanocrystals that are currently favoured for technological applications. [1] Corsini et al, J. Chem. Phys. 139,084117 (2013)

[1]Centre for Doctoral Training in Theory and Simulation of Materials Imperial College London via EPSRC grant

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