Exploring phase transformations in nanomaterials under pressure

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Nanocrystals show a wealth of distinctive behaviours with respect to their bulk counterparts, which can be tuned by varying their size, shape and surface. These include the way they respond to applied pressure and tensile stress, transforming from the original crystalline structure to new ordered or disordered phases. Of particular technological and fundamental interest are nanocrystals of tetrahedrally coordinated materials, such as Si, Ge, CdSe, CdS and ice, which can be driven by pressure toward highly coordinated crystalline or amorphous phases, and of TiO_2, which may show ferroelectric behaviour. To characterize the mechanisms of these phase transformations and explore the optical and electronic properties of the resulting systems, we have used a series of simulation techniques of different resolution, including density functional theory, molecular dynamics and the enhanced sampling method metadynamics, and developed specific protocols for nanomaterials under pressure. We have focussed, in particular, on the interplay between amorphization and crystallization, the effects of an implicit or explicit description of the environment, the emergence of metallic phases, piezochromic effects for pressure sensing, and the localization of soft modes that may trigger coherent phase transformations.