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Polarization Patterns In GeTe From Bulk To Ferroelectric Nanoclusters ENGIN DURGUN, University of Liege, RIAD SHALTAF, XAVIER GONZE, University of Catholic Louvain, PHILIPPE GHOSEZ, JEAN-YVES RATY, University of Liege — In this study, we investigated the ferroelectric and structural properties of GeTe crystal and nanoclusters, an alternative type of ferroelectric material, up to 1500 atoms from first-principles calculations based on density functional theory (DFT). Firstly, the dynamical, dielectric and elastic properties of GeTe in ferroelectric phase have been investigated [1]. Next, we demonstrate, for the first time at the DFT level, the existence in the interior of sufficiently large dots of polarization vortices giving rise to a net and reversible toroidal moment of polarization (G) [2]. The amplitude of G decreases with the size of the system and is totally suppressed below a critical diameter of 2.7 nm. The pattern of atomic distortions and the size evolution of the properties are discussed in relationship with the existence of a surface region within which the atoms behave differently. The validity of the results is checked for thicker structures with more layers and also for nanowires which can be considered as an infinite limit. (*)engin.durgun@ulg.ac.be
[1] R. Shaltaf, E. Durgun, J.-Y. Raty, Ph. Ghosez, and X. Gonze Phys. Rev. B 78, 205203 (2008) [2] E. Durgun, R. Shaltaf, J.-Y. Raty, X. Gonze, and Ph. Ghosez Nano. Lett. (submitted)

Engin Durgun
University of Liege

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