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Structure and electronic properties of GeTe nanoparticles from ab initio calculations.[1] GREGORY HAMMAD, ENS, Strasbourg, France, PHILIPPE GHOSEZ, JEAN-YVES RATY, University of Liege, Belgium — We use density functional theory to study the structure of small Ge-Te nanoparticles close to stoichiometry with various geometries. We particularly investigate the geometrical distortion of the rocksalt structure that gives rise to the ferroelectric effect in bulk GeTe. We observe that similar distortions appear in nanoparticles down to very small sizes (Ge15Te16). The electronic structure and the HOMO-LUMO states localization are shown to be in most cases related to the surface termination. Using linear response calculation (ABINIT code) we compute effective charges and compare these to the bulk value. We finally discuss the effect of the various factors (aspect ratio, facets, surface termination, stoichiometry) on the possibility that small (a few nm in size) Ge-Te nanoparticles could be ferroelectric.

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Jean-Yves Raty
University of Liege, Belgium

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