Abstract Submitted
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Ferroelectric Properties of TiO_2 Rutile Bulk and Surfaces Investigated by Ab Initio Calculations[1] ANNA GRÜNEBOHM, PETER ENTEL, Department of Physics, University Duisburg-Essen and CeNIDE, CLAUDE EDERER, School of Physics, Trinity College, Dublin — TiO_2 rutile is an incipient ferroelectric material [Lee et al., Phys. Rev. B **50**, 13379 (1994)] and theoretical studies have shown that a ferroelectric transition can be enforced [Montanari et al., J. Phys. Condens. Matter **16**, 273 (2004)]. The experimental realization of ferroelectric TiO_2 (110) surfaces would have great technical impact and already the tuning of the electric permittivity would be of interest, e.g., for optical coating. In order to get an insight into the ferroelectric trends, we have studied the atomic and electronic structure, as well as phonon spectra, dipolar interactions and the polarization, using density functional theory (VASP and PWscf). Accordingly, ferroelectric states polarized along (110) and (001) can be stabilized within bulk. We demonstrate the different strain dependencies of the corresponding polar modes, which opens up the possibility of strain engineering the polarization direction, and the resulting dielectric response [Grünebohm et al., Phys. Rev. B **84**, 132105 (2011) and Grünebohm et al. arxiv:1111.2575]. Although the dipolar interaction and the short range repulsion are both modified at the (110) surface, stable local dipoles are obtained within the surface planes, which increase with increasing strain.

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