Abstract Submitted
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Oxygen Vacancies in the Anatase (101) Surface: Formation Energies and Finite Size Effects[1] EDWARD TAIT, University of Cambridge, Department of Physics, CATERINA DUCATI, University of Cambridge, Department of Materials Science and Metallurgy, MIKE PAYNE, University of Cambridge, Department of Physics, NICHOLAS HINE, University of Warwick, Department of Physics — We present a study of oxygen vacancies in the anatase TiO_2 (101) surface. We take great care to minimise the impact of periodic boundary conditions on our results. We make use of the ONETEP[2] linear scaling DFT code to study defects in large (order 800 atom) simulation cells, to reduce long range strain interactions. We also make use of a scheme to correct for spurious periodic electrostatic interactions in the case of charged defects[3]. Finally we study the behaviour of defect formation energies as a function of distance from the surface, and demonstrate convergence to bulk formation energies with depth. We also present novel functionality for EELS calculations within LS-DFT, suitable for large nanomaterials systems.

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[2]Skylaris C K, Haynes P D, Mostofi A A and Payne M C 2005 *J. Chem. Phys* **122**
[3]Komsa, H-P and Pasquarello A 2013 *Phys. Rev. Lett.* **110**:095505

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