Large Scale and Linear Scaling DFT and its applications to polarisation textures in $PbTiO_3$ thin films

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We will survey the underlying theory behind the large-scale and linear scaling DFT code, CONQUEST[1], which shows exceptional parallel scaling (demonstrated up to 200,000 cores) and can be applied to up to ten thousand atoms with diagonalisation, and millions of atoms with linear scaling. We will give details of the representation of the density matrix and the approach to finding the ground state, and discuss the implementation of molecular dynamics with linear scaling. We will give an overview of the performance of the code, and provide examples of recent developments.

We will also discuss the recent application of CONQUEST to complex ferroelectric systems with up to 5,000 atoms[2,3]. In Fig. 1(a) and (b), the local polarisation textures[2] of $PbTiO_3$ thin films on $SrTiO_3$ are shown for 9 layers (top) and 3 layers (bottom). The formation of polar vortices is clear in the thick film, while the thinner film cannot support these, instead showing a polar wave with chiral bubbles forming at the surface; we have extended these studies using linear scaling to investigate the interaction of domain walls with surface trenches[3].

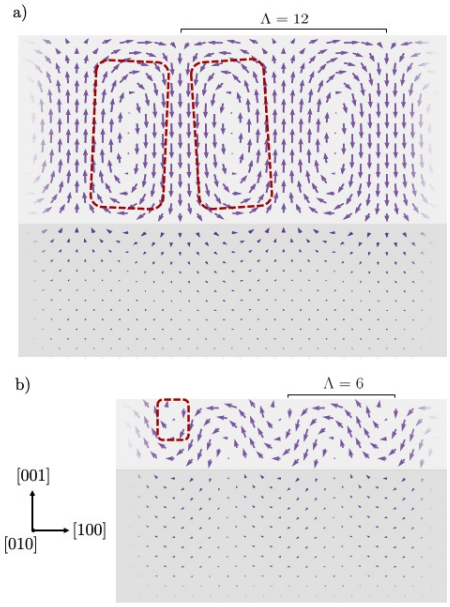

Figure 1. Local polarisation in $PbTiO_3$ films on $SrTiO_3$: (a) 9 layers of PTO; (b) 3 layers.

References

1. A. Nakata *et al.*, *J. Chem. Phys.* **2020** *152*, 164112
2. J. S. Baker and D. R. Bowler, *Adv. Theory Simul.* **2020** *3*, 2000154
3. J. S. Baker and D. R. Bowler, *Phys. Rev. Lett.* **2021** *127*, 247601