Abstract Submitted
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Recovering hidden Bloch character: Unfolding Electrons, Phonons, and Slabs[1] PHILIP B. ALLEN, Stony Brook University, TOM BERLIJN, University of Florida, DAVID CASAVANT, University of Maryland, JOSE SOLER, Universidad Autonoma de Madrid — One of the main problems of first principles supercell calculations is the band folding problem. As the supercell gets larger, the bands get folded into a smaller Brillouin zone and cease to give information about the Bloch character of the underlying normal cell. To tackle this problem an unfolding formalism has been implemented in first principles calculations via several techniques [1-5]. Here we will present an extended unfolding formalism for finite systems and exemplify it with first principles calculations of a Si (111) slab.

[1] S. Baroni et al, PRL 65, 84 (1990)
[2] F. Giustino et al, PRL 98, 047005 (2007)
[3] W. Ku et al, PRL 104, 216401 (2010)
[4] V. Popescu et al, PRL 104, 236403 (2010)
[5] M. W. Haverkort, arXiv:1109.4036

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