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Finite-size correction scheme for supercell calculations in Dirac-point two-dimensional materials

Modern electronic structure calculations are predominantly implemented within the super cell representation in which unit cells are periodically arranged in space. Even in the case of non-crystalline materials, defect-embedded unit cells are commonly used to describe doped structures. However, this type of computation becomes prohibitively demanding when convergence rates are sufciently slow and may require calculations with very large unit cells. We have shown [1] that a hitherto unexplored feature displayed by several 2D materials may be used to achieve convergence in formation- and adsorption-energy calculations with relatively small unit-cell sizes. The generality of our method is illustrated with Density Functional Theory calculations for diferent 2D hosts doped with diferent impurities, all of which providing accuracy levels that would otherwise require enormously large unit cells. This approach provides an efcient route to calculating the physical properties of 2D systems in general but is particularly suitable for Dirac-point materials doped with impurities that break their sublattice symmetry.

References

[1] C.G. Rocha, A. R. Rocha, J. H. Garcia, P. Venezuela and M. S. Ferreira, Scientifica Reports, 8 (2018) 9348.