Multi-scale approach for strain engineering of single-layer phosphorene

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One of the many features of atomically thin materials is the possibility to engineer their properties using deformations. Semiconducting materials, like phosphorene, are of particular interest due to their potential for optoelectronic applications.
The theoretical description of the electromechanical behaviour requires a consistent treatment of electronics and mechanics. In this spirit, a multi-scale approach is presented, which combines a recently developed valence-force model [1] - relating macroscopic strain to microscopic displacements of atoms [2] - and a tight-binding model [3] with distance-dependent hopping parameters to obtain strain-induced electronic properties. The resulting self-consistent electromechanical model is suitable for large-scale modelling of phosphorene devices. We demonstrate this for the case of an inhomogeneously deformed phosphorene drum, which may be used as an exciton funnel [4].

References

[1] D. Midtvedt and A. Croy, Phys. Chem. Chem. Phys. 18, 23312 (2016).
[2] D. Midtvedt, C. H. Lewenkopf, and A. Croy, 2D Materials 3, 011005 (2016).
[3] A. N. Rudenko, S. Yuan, and M. I. Katsnelson, Phys. Rev. B 92, 085419 (2015).
[4] P. San-Jose et al, Phys. Rev. X 6, 031046 (2016).

Figures

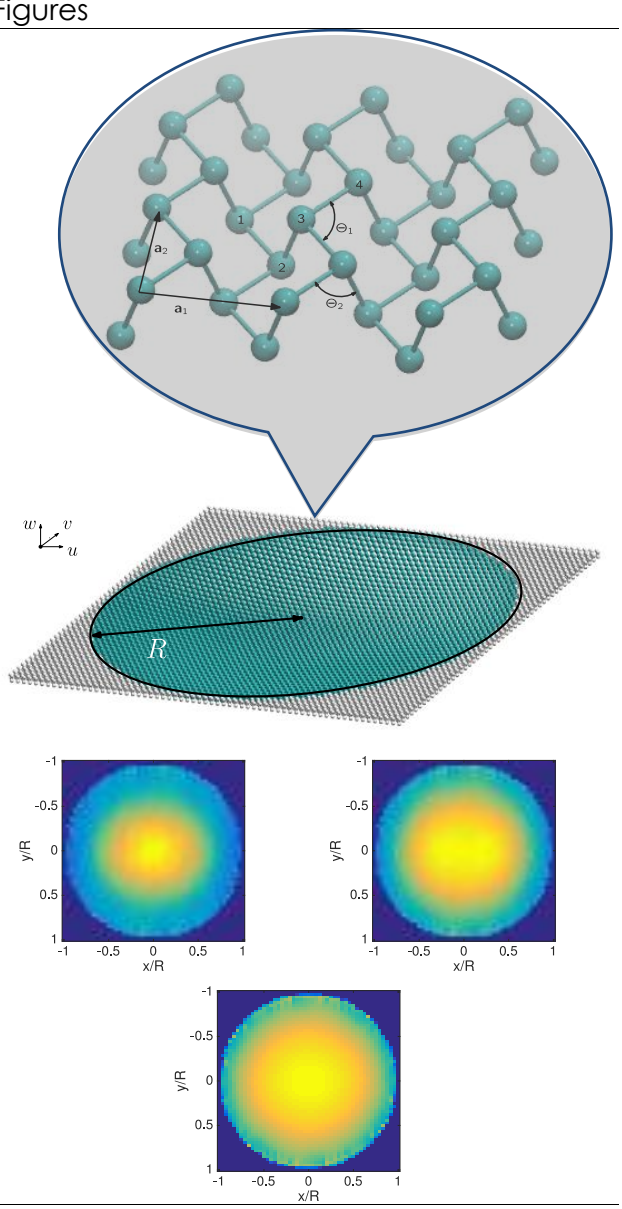

Figure 1: Sketch of phosphorene structure (topmost). Pressurized phosphorene drum (middle) and maps of the local band-gap (bottom) induced by the deformation at different pressures.