Chiral surface Moiré superlattices formed with epitaxial 2D materials

Xue-Sen Wang
Department of Physics, National University of Singapore
2 Science Drive 3, Singapore 117542
phywxs@nus.edu.sg

Crystal surfaces with chiral Moiré superlattices not only possess special electronic, magnetic and optoelectronic properties attributed to the Moiré superstructures [1,2] and surface chirality [3,4] individually, but also could host novel phenomena induced by the coupling of these two structural features. Here, we explore the chiral Moiré superlattices formed on crystal surfaces when they are covered with epitaxial 2D atomic layers. It has been demonstrated that when a 2D atomic layer (e.g., graphene, blue phosphorene [5]) is grown on a crystal surface with a lattice mismatch, a Moiré superlattice can be observed. Depending on the strength of bonding between the 2D atomic layer and the substrate surface, and the atomic density of the 2D layer, the period of the Moiré superlattice can be adjusted in certain range. Furthermore, when the bonding with the 2D layer is strong enough, the top atomic layer of the substrate may undergo a substantial reconstruction as a way of elastic relaxation. As illustrated in the case of blue phosphorene grown on a Cu(111) substrate [5], such an elastic relaxation can result in a chiral Moiré superlattice. While the electronic density optimization plays an important role in the long-period reconstruction of Cu(111) surface, such substrate top-layer reconstruction is plausible also on the surface of a 3D layered crystal (such as graphite, TMDC, or group-IV monochalcogenide (e.g., SnSe)) relative strongly bound with an epitaxial 2D atomic layer. Combining computational and experimental studies, we can explore such heteroepitaxial Moiré superstructures of various 2D overlayers grown on 3D layered crystals. With lattice mismatch, interlayer bond strength, overlayer thickness (i.e., monolayer to few-layers) and the material properties of the building blocks as the tuning nobs, this will allow us discover more Moiré superlattices, some of them chiral, with novel properties for different applications.

References

[1] D. M. Kennes *et al*., Moiré heterostructures as a condensed-matter quantum simulator. Nat. Phys. 17 (2021) 155.
[2] L. Du, M. R. Molas, Z. Huang, G. Zhang, F. Wang, Z. Sun, Moiré photonics and optoelectronics, Science 379 (2023) 1313.
[3] S. J. Jenkins, Chirality at Solid Surfaces (Wiley, Hoboken, NJ, 2018).
[4] G. Chang *et al*., Topological quantum properties of chiral crystals, Nat. Mater. 17 (2018) 978.
[5] Y.-H. Song, M.U. Muzaffar, Q. Wang, Y. Wang, Y. Jia, P. Cui, W. Zhang, X.-S. Wang, Z. Zhang, Realization of large-area ultraflat chiral blue phosphorene, Nat. Commun. 15 (2024) 1157.