Moiré superlattice networks in twistronics bilayers of transition metal dichalcogenides

Vladimir Fal'ko
[1] *National Graphene Institute, University of Manchester, Booth Street East, Manchester M139PL, UK*
[2] *Henry Royce Institute for Advanced Materials, Oxford Road, Manchester M139PL, UK*
vladimir.falko@manchester.ac.uk

We apply a multiscale modelling approach to study moiré superlattice in twisted homo- and heterobilayers of transition metal dichalcogenides (TMD), taking into account the interlayer hybridisation of the electronic orbital and lattice reconstruction due to stacking-dependent adhesion. First of all, we develop DFT-parametrized interpolation formulae for interlayer adhesion energies of $MoSe_2$, WSe_2, MoS_2, and WS_2 with both parallel and antiparallel orientation of their unit cells and arbitrary offset of the honeycomb lattices in the adjacent layers [1,2]. Then, we combine those interpolation formulae with elasticity theory and analyze the bilayer lattice relaxation into mesoscale domain structures. We find that 3R and 2H stacking domains develop for, respectively, bilayers with parallel (P) and antiparallel (AP) orientation of the monolayer unit cells, separated by a network of dislocations, for twist angles $\theta < \theta_P \sim 2.5$ and $\theta < \theta_{AP} \sim 1$. Such lattice reconstruction has been verified by STEM imaging [2]. We also show that the triangular domain structures of P-oriented homobilayers would manifest itself in local tunnelling characteristics of marginally twisted bilayers [1,2]: these domains feature the layer asymmetry of band-edge wave functions and also the ferroeletric interlayer polarisation. For AP bilayer, we show that the deformation of the lattices around domain walls (which resemble twist dislocations oriented along the planes of in bulk 2H crystals) generate piezo-electric charges [1], reaching local density up to $\pm 0.5 \times 10^{12} e/cm^2$ at the junctions of the honeycomb domain wall network, whereas the 3R stacking domains in P-bilayers feature weak ferroelectric (interlayer) charge transfer [3,4]. Finally, we use DFT modelling of bandstructure of bilayers with various stacking configurations and interlayer distances to develop and parametrise **k·p** theory Hamiltonians in the relevant parts of the Brillouin zone, and, then, establish the electronic structure of the bilayer across the moire supercell, taking into account the ferroelectric and piezolectric charge transfers [5].

REFERENCES

[1] V. V. Enaldiev, V. Zólyomi, C. Yelgel, S. J. Magorrian, and V. I. Fal'ko, Phys. Rev. Lett. 124, 206101 (2020).
[2] A. Weston, Y. Zou, V. Enaldiev, A. Summerfield, N. Clark, V. Zolyomi, A. Graham, C. Yelgel, S. Magorrian, M. Zhou, J. Zultak, D. Hopkinson, A. Barinov, T. Bointon, A. Kretinin, N.R. Wilson, P.H. Beton, V.I. Fal'ko, S.J. Haigh, R. Gorbachev, Nature Nanotechnology 15, 592 (2020)
[3] V. Enaldiev, F. Ferreira, S. Magorrian, V. Fal'ko, 2D Mater 8, 025030 (2020)
[4] F. Ferreira, V. Enaldiev, V. Fal'ko, S. Magorrian - arXiv:2103.06093
[5] F. Ferreira, S. Magorrian, V. Enaldiev, D. Ruiz-Tijerina, V. Fal'ko - arXiv:2103.06320

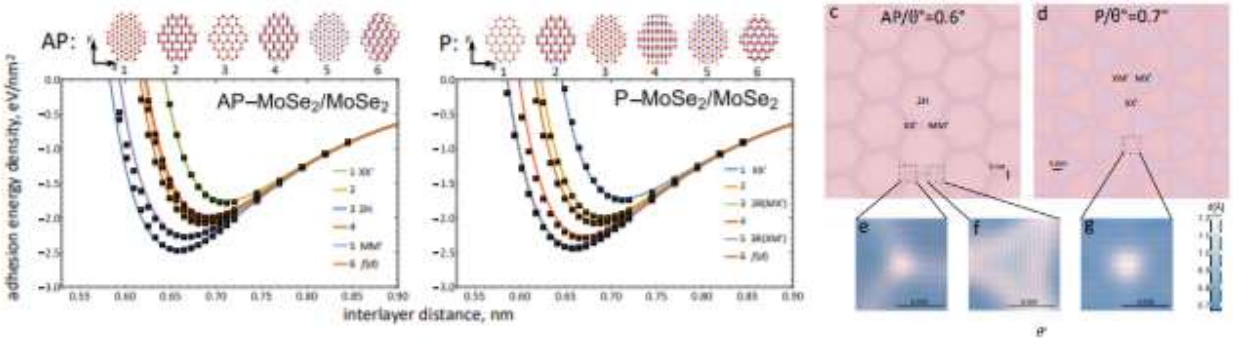

Figure: (Left) Interlayer distance dependence of adhesion energy for various stacking configurations of P- and AP-bilayers. (Right) Domain wall network in twisted bilayers due to the growth of 3R (for P) 2H (for AP) domains.