Valley Jahn-Teller effect in twisted bilayer graphene

Mattia Angeli
Erio Tosatti and Michele Fabrizio

International school for advanced studies (SISSA), Via Bonomea, 265, 34136 Trieste TS

mangeli@sissa.it

The surprising insulating and superconducting states of narrow-band graphene twisted bilayers have been mostly discussed so far in terms of strong electron correlation, with little or no attention to phonons and electron-phonon effects. We found that, among the 33492 phonons of a fully relaxed θ=1.08 twisted bilayer, there are few special, hard and nearly dispersionless modes that resemble global vibrations of the moirè supercell, as if it were a single, ultralarge molecule. One of them, doubly degenerate at Γ with symmetry A1+B1, couples very strongly with the valley degrees of freedom, also doubly degenerate, realizing a so-called Exe Jahn-Teller (JT) coupling. The JT coupling lifts very efficiently all degeneracies which arise from the valley symmetry, and may lead, for an average atomic displacement as small as 0.5 mA, to an insulating state at charge neutrality.

This insulator possesses a non-trivial topology testified by the odd winding of the Wilson loop. In addition, freezing the same phonon at a zone boundary point brings about insulating states at most integer occupancies of the four ultra-flat electronic bands. Following that line, we further study the properties of the superconducting state that might be stabilized by these modes. Since the JT coupling modulates the hopping between AB and BA stacked regions, pairing occurs in the spin-singlet Cooper channel at the inter-(AB-BA) scale, which may condense a superconducting order parameter in the extended s-wave and/or d + id-wave symmetry.

References

[1] M. Angeli, E. Tosatti, M. Fabrizio, arXiv:1904.06301

[2] M. Angeli, D. Mandelli, A. Valli, A. Amaricci, M. Capone, E. Tosatti, and M. Fabrizio, Phys. Rev. B **98**, 235137

Figures

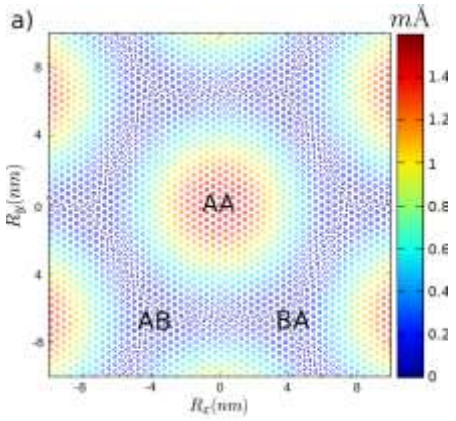

Figure 1: a): atomic displacements on one of the two layers corresponding to the A1-symmetry phonon mode. The direction of displacement is represented by a small arrow centered at each atomic position, while its modulus is encoded in colors.

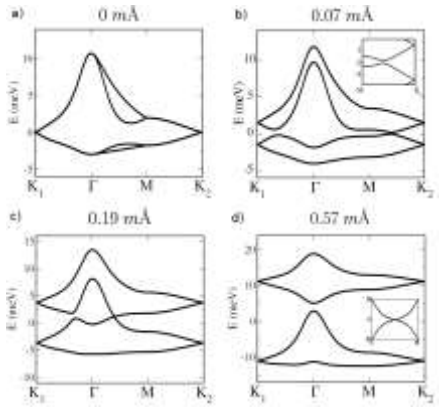

Figure 2: a): Evolution of the FBs when the lattice is distorted with increasing intensity along the mode in Fig. 1. Panel (a) undistorted. Panel(b) mean displacement per atom 0.07 mÅ. (c) mean displacement 0.19 mÅ. Panel (d) mean dis-placement 0.57 mÅ. Inset:Wilson loop of the lowest two bands in panel