Moire bands and electronic properties of graphene on hexagonal boron nitride

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Abstract

When atomically thin two-dimensional materials are layered, they often form incommensurate noncrystalline structures that exhibit long-period moire patterns when examined by scanning probes. In this talk I present a methodology that uses information obtained from *ab initio* calculations performed on short-period crystalline structures to derive effective Hamiltonians that are able to efficiently describe the influence of the moire pattern superlattices on electronic properties. We applied our approach to obtain the Hamiltonian of graphene on hexagonal boron nitride (G/BN) that can be used to calculate electronic properties of interest for arbitrary twist angles and lattice constants. We show that our multiscale approach can be used to obtain electronic structure models that have predictive accuracy, and that moire strains can play an important role in reconfiguring the mechanical and electronic properties of G/BN such as its band gap. The bridge between the continuum and the lattice Hamiltonian established by our theory can be used in realistic simulations of G/BN subject to disorder or perpendicular magnetic fields.

[1] J. Jung, A. Raoux, Z.H. Qiao and A. H. MacDonald, ‘Ab-Initio Theory of Moiré Superlattice Bands in Layered Two-Dimensional Materials’, Physical Review B 89, 205414 (2014).
[2] J. Jung, A. DaSilva, A. H. MacDonald, and S. Adam, ‘Origin of band gaps in graphene on hexagonal boron nitride’, Nature Communications 6:6308 (2015).
[3] N. Leconte, A. Ferreira, and J. Jung, ‘Efficient multiscale lattice simulations of strained and disordered graphene’, Chapter 2 of 'Semiconductors and semimetals, 2D materials’, Elsevier 2016.

About the Speaker

Jeil Jung is an associate professor at the University of Seoul at Seoul, Republic of Korea. He received his Ph.D. degree in UNED in Madrid, Spain in 2005. From 2006 to 2013, he worked as a Fulbright research fellow and lecturer in the University of Texas at Austin, collaborating with Prof. Allan MacDonald. From 2013 to 2014 he worked as a Senior Research Fellow at the National University of Singapore, collaborating with Prof. Shaffique Adam, before joining the faculty of University of Seoul in 2015. He is working in the field of condensed matter theory, with a focus in the development of exchange-correlation functionals in density functional theory and electron-electron interactions in graphene. He has published 43 articles with 4 in Nature Communications, 1 in Nature Nanotechnology and 5 in Physical Review Letters. He has a Hirsch index of 20 and a total number of citations over 1500 (Google scholar).