Mesoscopic modeling of 2D materials & heterostructures

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The study of the physical properties of 2D materials requires the crossover from the microscopic to the mesocopic regime where new phenomena emerge. Furthermore, when one wants to study combinations of different materials with a different orientation with respect to each other, the unit cells can already contain thousands of atoms. This makes it impossible to study electronic properties using traditional methods such as density functional theory (DFT).
Here we will give an overview of our tight-binding propagation method (see e.g. [1] and [2]), which can be used to calculate electronic, optical and transport properties of systems with millions of atoms. More importantly, we will show our results of the study of moiré patterns in graphene-based heterostructes such as graphene/hBN [3], graphene/Ru [4] and twisted trilayer graphene [5].

References

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[2] S. Yuan, R. Roldán, M.I. Katsnelson, Phys. Rev. B 84, 035439 (2011)
[3] G.J. Slotman, M.M. van Wijk, P.L. Zhao, A. Fasolino, M.I. Katsnelson, S. Yuan, Phys. Rev. Let. 115 186801 (2015)
[4] A. Politano, G.J. Slotman, R. Roldán, G. Chiarello, D. Campi, M.I. Katsnelson, S. Yuan, 2D Materials 4 (2), 021001 (2017)
[5] Q. Yao *et al.* (submitted)

Figures

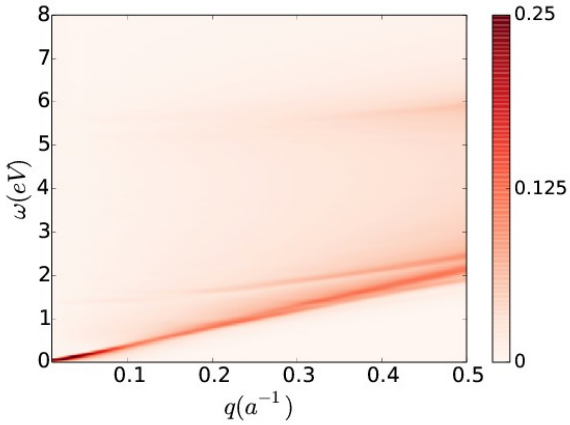

Figure 1: A contour plot of the imaginary part of the dynamical polarization $\Im\Pi(q,\omega)$ for graphene on ruthenium. [4]

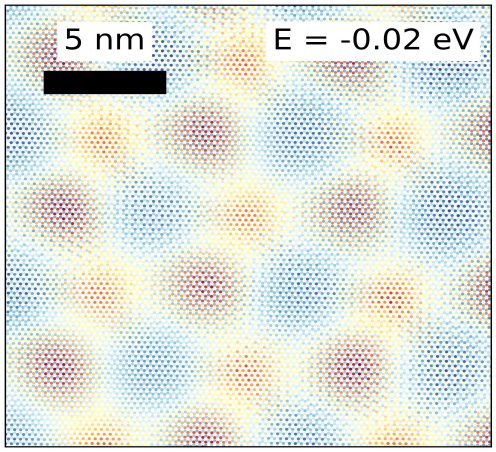

Figure 2: Calculated LDOS for trilayer rotated graphene. [5]