Correlation effects on topological end-states in finite-size armchair graphene nanoribbons

Antoine Honet[1]
Luc Henrard[1]
Vincent Meunier[2]
[1]*Department of Physics and Namur Institute of Structured Materials, University of Namur, Rue de Bruxelles 51, 5000 Namur, Belgium*
[2]*Department of Engineering Science and Mechanics, The Pennsylvania State University, University Park, PA, USA*
antoine.honet@unamur.be

Finite-size armchair graphene nanoribbons are expected to host topological states that are spatially located at the two zigzag ends of the ribbons (see fig.1). The number of topological states is predicted by topological invariant defined for periodic ribbons and depends on the number of carbon atoms in the ribbons' width. These classifications on the ribbons' width rely most often on topological invariant evaluation based on tight-binding Hamiltonian models, i.e. with no interaction between electrons [1, 2, 3]. One can include interaction on top of a tight-binding models by inserting new terms in the model Hamiltonian and adopting the Hubbard Hamiltonian. This model is a well-known model to describe graphene and graphene nanofragments but is often treated in a mean-field approximation. In this approximation, each electron interacts with a mean-field resulting from all the electrons. No direct two-electron interactions are accounted for and the correlation is neglected. Treating the Hubbard model with the exact interaction terms and the total interaction for a system with more than a few tens of electrons is currently intractable from a numerical point of view. In-between approximations – restoring a part of the correlation but numerically tractable – are thus important. In this study, we investigated in more details the so-called GW approximation [4, 5, 6]. In particular, we investigated how this correlation impacts the topological end-states in graphene nanoribbons and show how their energies or spatial properties are affected. We also compare our results to published experimental data, showing a greater agreement when correlation effects are included.

References

[1] T. Cao, F. Zhao, and S. G. Louie, Phys. Rev. Lett. ,119(7), 2017.
[2] M. P. López-Sancho and M. C. Muñoz, Phys. Rev. B , 104(24), 2021.
[3] J. Jiang and S. G. Louie, Nano Lett., 21(1), 2021.
[4] J.-P. Joost, A.-P. Jauho and M. Bonitz, Nano Lett., 19(12), 2019.
[5] A. Honet, L. Henrard, and V. Meunier, Carbon Trends, 4, 2021.
[6] A. Honet, L. Henrard, and V. Meunier, AIP Advanced, 12(3), 2022.

Figures

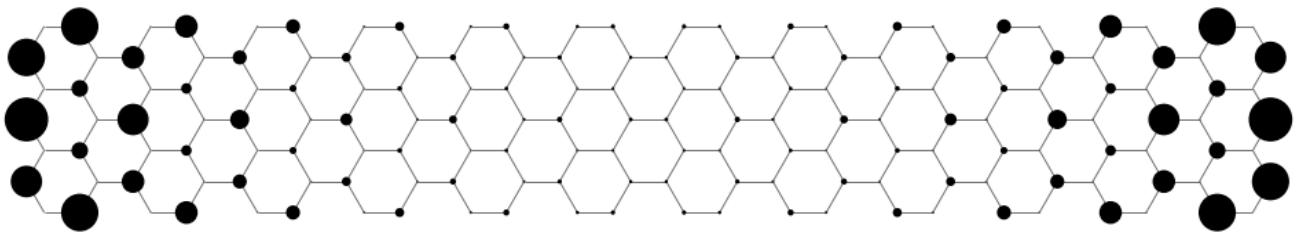

Figure 1: Electronic density of a topological end-states in a 7-atom width armchair graphene nanoribbon. The size of the dots is proportional to the mean densities of electrons.