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Project title: Extreme light-matter interactions in low dimensional materials

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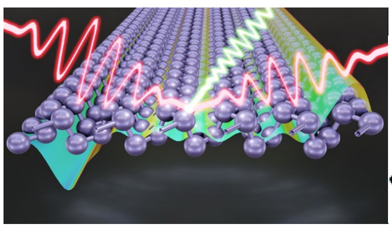
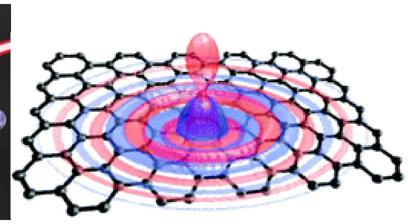
PROJECT DESCRIPTION:

The isolation of graphene, the atomically-thin carbon layer, has triggered extensive interdisciplinary research efforts to capitalize on its many fascinating electronic, mechanical, and optical properties for emerging new technologies [1], and has launched investigations into other promising two-dimensional materials and their heterostructures that are further catalyzed by novel physics and steady progress in nanofabrication technology [2]. Despite its atomic-scale thickness, pristine graphene offers a relatively large light-matter interaction associated with the optical excitation of electrons from its populated valence band to the unpopulated conduction band, both of which have a peculiar conical shape that gives rise to a remarkable universal 2.3% absorption over a broad range of optical wavelengths. Even more enticing is the ability to electrically tune graphene from semiconducting to metallic states, ultimately enabling control of light excitation pathways within a single-atom-thick material [3].

The objective of this project is to theoretically explore other 2D materials using a newly developed tight-binding based formalism.[4] The project will consist of three phases; in the first phase a small group of promising 2D materials candidates will be identified by looking through relevant literature and material databases. The second part will be to create a tight-binding representation of the chosen materials using maximally localized Wannier functions.[5] Once the models have been created, the final part of the project will be concerned with exploring the extreme nonlinear optical response using the already developed software and possibly identifying novel material candidates for applications within nonlinear optics.

[1] A. K. Geim, Science **324**, 1530 (2012).
[2] T. Low et al., Nat. Mater. **16**, 182 (2017).
[3] C.-F. Chen et al., Nature **471**, 617 (2011).
[4] L. Jelver and J. D. Cox, Nonlinear Plasmonics in Nanostructured Phosphorene, ACS Nano 17, 20043 (2023).
[5] N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, and D. Vanderbilt, Maximally Localized Wannier Functions: Theory and Applications, Rev. Mod. Phys. 84, 1419 (2012).