GRANAD – framework and code for optoelectronic properties of low-dimensional structures

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Low-dimensional structures like 1D atomic chains and 2D nanoflakes have unique electronic, optical, and material properties due to their chemical composition and geometry. They can be used as elementary building blocks in heterostructures realizing nanoscaled optoelectronics tuned by electronic or optical means or in the presence of atomic defects (adatoms) [1]. In reverse, a flake or chain can be exploited to modulate the dynamics of adatoms positioned in its vicinity [2]. We have developed a theoretical framework and a related Python toolbox, GRANAD (Graphene Nanoantennas with ADatoms) [3], to study these properties. The framework combines a tight-binding approach to model the electronic properties of 2D nanoflakes with the master equation approach to capture electron dynamics. The single-electron model allows for a favorable linear scaling of the Hilbert space size with the number of carbon sites, allowing us to study relatively large flakes. Originally developed to model graphene, the code has recently been extended to include different 2D materials and their stacks. I am going to present the capabilities of the GRANAD toolbox and the selected results we have obtained. In particular, the framework has been recently applied to investigate the nature of plasmonic excitations on graphene nanoflakes [4] or the influence of atomic defects on the optical properties of low-dimensional material structures [1, 2], including spontaneous emission of light from dipolar adatoms near atomic chains (Figure 1).

References

[1] M. M. Müller, et.al., Phys. Rev. B 104, 235414 (2021).
[2] M. Kosik et.al., Nanophotonics, 11, 3281-3298 (2022).
[3] D. Dams, et.al., Submitted to Comp. Phys. Commun.
[4] M. M. Müller, et.al., J. Phys. Chem. C 124, 24331–24343 (2020).

Figures

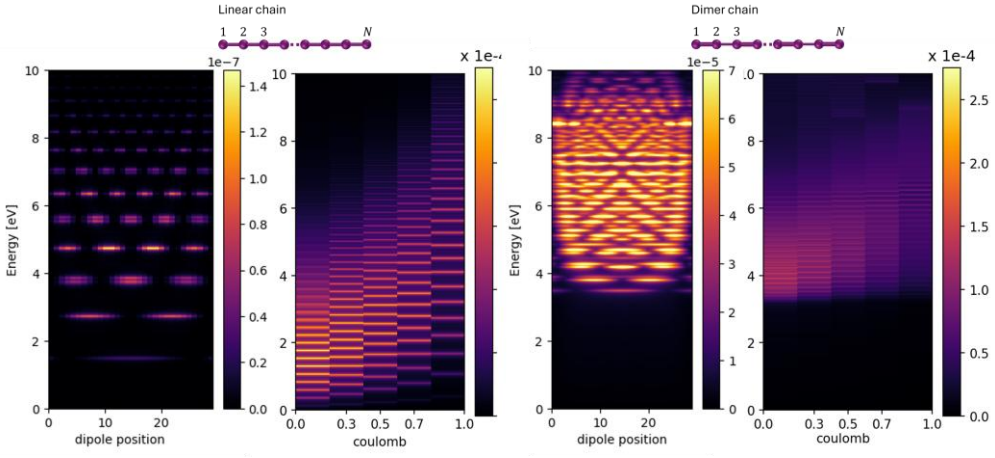

Figure 1: Comparison of response in the case of the dipolar atom near the 30-atom linear and dimer chains - imaginary part of the Green's function at the dipole's position, characterizing the spontaneous emission rate as a function of the dipole position and Coulomb interaction strength.