Novel 2D materials for opto-electronic applications: insight from parameter-free quantum-mechanical methods

Maurizia PALUMMO

INFN and Dipartimento di Fisica Università di Roma "Tor Vergata"
Via della Ricerca scientifica 1 00133 Rome Italy

The use of emerging two-dimensional and layered materials in technological applications presupposes a detailed knowledge of their chemical and physical properties and, in this context, ab initio theoretical methods are playing a fundamenla role.
Among the large number of 2D materials discovered after graphene, of particular interest for opto electronic applications is the family of Transition Metal Dichalcogenides (TMDs) and more recently that one of layered Ruddlesden Popper organic-inorganic halide perovskites (RPPs).
The aim of my talk is to show how the use of parameter free atomistic simulations can contribute to improve the microscopic understanding of the opto-electronic properties of these two classes of novel 2D materials and to predict new ones. I will show how ab--initio DFT and post-DFT simulations based on Many-Body Green Function approach, provide a very useful scheme to explain:
i) the giant electronic bandgaps renormalization ii) the strong light-matter interaction iii) the presence of strongly bound excitons. I will also discuss how to calculate in a fully ab-initio framework the exciton radiative lifetimes and the influence of electron-phonon interaction on the electronic and optical spectra.
Finally for 2D-TMDs I will show how doping and molecular functionalization can tune their opto-electronic properties.