Ab initio 2d material design for sustainable applications

The evolution of technologies for environmentally friendly applications is deeply intertwined with research activities on material exploration and design, both in the laboratory and *in silico.* I will present key examples in which atomistic simulations proved fruitful in explaining and predicting properties of 2d materials for sustainable technologies. Density Functional Theory and many-body perturbation theory were successfully applied to hot fields such as electrocatalysis, with the development of new 2d carbon-based single atom catalysts, photocatalysis, by studying the exciton lifetimes of graphitic carbon nitride, photovoltaics, with the proposal of new ultrathin heterostructures based on transition metal dichalcogenides and, eventually, water treatment, by expanding the studies on porous graphene membranes. From all these examples, it will emerge how theoretical methods can provide valuable results to better interpret and guide the experimental activity.