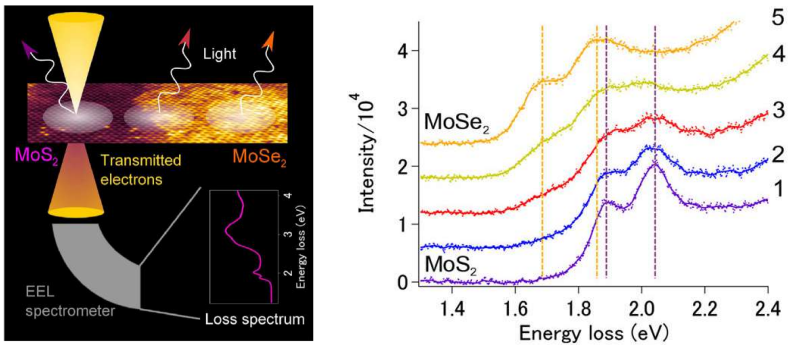
Embedding method for excitons at the interface in 2D lateral heterostructures

Project description: Despite the intense experimental activity, excitations in 2D heterostructures are a severe challenge for modelling and first-principle simulations. In fact, for predictions to be quantitative, one must treat on the same footing long-range interactions (e.g. dielectric screening, magnetic ordering) and short-range ones (in particular, the hybridization across interfaces with possibly complex morphology). This is particularly true for lateral heterostructures. These are formed of 2D layers connected side-by-side.

Ab-initio solution of the Bethe-Salpeter equation gives accurate dielectric properties and optical spectra, but it can be hardly done on simulation cells encompassing more than few tens of atoms. On the other hand, semi-empirical approaches like tight-binding are so light that can be applied to systems of thousands of atoms, but the accuracy of the results depends on the physical content of the model itself and on a delicate parametrization procedure. The ideal scenario would be that of adopting a double-framework approach taking the best from each theory.



Observation of the evolution of an exciton across the interface of a MoS2/MoSe2 lateral heterostructure.
Images taken from Phys. Rev. Lett. ***114****, 107601 (2015)*

A powerful way to do that is through embedding methods. They provide a rigorous framework to include long-range information inside an accurate local calculation. Such methods are used routinely in several domains, including quantum transport simulations. In a typical quantum-transport simulation, some current passes through a system (typically a molecule) attached to two metallic terminals. Non-Equilibrium Green functions are used to calculated the current flow through the molecule while the influence of the terminals is taken into account through lead self-energies derived, e.g., from tight-binding models. Ideally, if in this scheme one replaces the terminals with two 2D materials and the target system with an interface exciton, the scenario will become the one tackled by this project where an equilibrium Green's function theory (ab-initio Bethe-Salpeter) would be solved instead of a non-equilibrium one.

The projects aims at investigating an almost unexplored physics (electronic excitations at linear interfaces) by the development of a novel embedding method, inspired by quantum transport techniques, and designed to tackle specifically electron-hole excitations at the 1D heterojunctions of lateral heterostructures.

Job description: Post-doc position 24 months from January or February 2024

Academic level: Ph.D. in Physics

Location: LEM, Châtillon, France

Expertise: Any among ab-initio Bethe-Salpeter equation, ab-initio quantum transport and tight-binding modelling. Proven skills in numerical implementation. The more are met, the better.

Application: send your CV with publication list, a motivation letter and provide at least two references to *lorenzo.sponza@onera.fr*