

Post-doctoral position in theory and atomistic simulation

“Excitonic properties of structurally inhomogeneous 2D materials”

A **24 month post-doctoral position** is open in a **joint research program** gathering the *Service de Physique de l'Etat Condensé* at CEA-Saclay (first 12 months) and the *Laboratoire d'Etude des Microstructures* at Onera-Châtillon (second half of the position). Both are located in the Paris area, France.

Subject description:

Since graphene takeoff in the 2000's, the field of two-dimensional systems has been gradually enriched by new materials, such as hexagonal boron nitride, dichalcogenides or black phosphorus. Despite the progress done in the investigation of the fundamental properties of these materials and their heterostructures, the door is still wide open to explore new effects with active 2D materials. In particular, these nearly zero thickness materials exhibit novel mechanisms to generate, detect, broadcast and control optical signals with possible technological applications in photonics, light harvesting, signal processing, and alike.

In this project, optical properties of different 2D materials will be studied at the atomic scale using computer simulations. The theoretical framework will rely on many-body equations describing the electronic structure and its excitations, in particular the excitonic effects (the Bethe-Salpeter equation). The equations will be solved by means of *ab initio* simulation packages (for instance Quantum Espresso and Yambo) and appropriate tight-binding models which provide physical insight and can be easily extended to complex morphologies (defects, interfaces, deformations, disorder). Questions to be addressed concern the calculation and analysis of the excitonic properties of twisted hBN bilayers and graphene-based anti-dot lattices. The development of the project will be carried out in close collaboration with experimental partners.

Skill requirements and experience:

Applicants should hold a Ph.D. degree in condensed matter physics, materials science or physical chemistry by less than one year. Strong experience in the use of standard *ab initio* software and/or tight-binding models is mandatory, with an interest in optical response calculations (RPA and beyond, BSE,...). We also prioritize candidates with experience in code development and modeling. The total duration of previous post-doctoral contracts can not exceed one year.

Application procedure:

Qualified candidates should send their curriculum vitae, the list of publications and a description of their research experience and interests to sylvain.latil@cea.fr and lorenzo.sponza@onera.fr.