Computational Optimization of Optoelectronic and Transport Properties in Defected 2D Materials

In the realm of cutting-edge materials science and nanotechnology, the pursuit of enhancing optoelectronic and transport properties in two-dimensional materials is a paramount research effort. Defects, which can arise from various sources such as impurities, vacancies, or structural irregularities, have a profound impact on the optoelectronic properties of materials. In many cases, controlling and manipulating defects is not just desirable but essential for optimizing the performance of electronic devices. This is particularly true for 2D materials like Transition Metal Dichalcogenides (TMDs), which are known for their sensitivity to defects. The computational approach employed in this research will span a large spectrum of techniques, including Density Functional Theory, many-body perturbation theory, and the Boltzmann transport model. By combining these computational approaches, this project aims at a comprehensive understanding of how defects influence the optoelectronic and transport properties of TMDs.
Collaboration with the experimental labs at CNR-Trento, as partner of the PRIN2022 project "2D-EMMA", will foster a tightly integrated and stimulating exchange between theoretical predictions and experimental results.

The researcher will perform calculations with various ab-initio codes, such as Quantum ESPRESSO, YAMBO and PERTURBO, to elucidate the transport mechanisms and the optoelectronic properties of the systems produced at CNR-Trento. Key objectives involve, for instance: studying transport in TMD MLs with defects, evaluating the effect of a substrate (e.g. Si/SiO2) on the properties of the MLs, assessing the optoelectronic properties of amorphous thin films of TMDs, studying the interaction with gas molecules for gas-sensing applications.