Two-Dimensional Semiconductor Doping via Molecular Charge Transfer

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Among the various types of two-dimensional materials, transition metal dichalcogenides (TMD) represent one of the most interesting families from a technological point of view, as they have gaps of the order of 1-3 eV. This property makes them excellent supports for the manufacture of transistors, photovoltaic cells and more generally optoelectronic devices. Furthermore, TMDs are among the most studied materials due to their quantum properties and functionalities which make them particularly suitable for possible applications in quantum technologies. Hybrid materials (obtained for example by combining organic films with TMD substrates) provide further extended possibilities to design and develop new materials with specific functionalities necessary for the realization of quantum devices. The doctoral project, therefore, fits fully into the theme "Quantum science and technology" of the PNRR. The PhD student's research activity will be developed in synergy with the Italian PNRR extended partnership project "National Quantum Science and Technology Institute" (NQSTI).

TMDs are composed of three atomic layers in the form X-M-X, where two atomic planes of group 16 elements (X) are separated by a plane of transition metal atoms (M), and can be found in monolayer crystals in the form of MX2 units stacked and weakly interacting with each other. Considering the large number of possible combinations of chalcogens and transition metals it is evident that the different TMDs can offer a wide range of electronic, optical and chemical properties without resorting to further functionalizations. However, despite the apparent advantages of TMDs and several years of research aimed at improving the efficiency of devices based on these materials, their efficiency continues to be inferior to their silicon-based counterparts. One of the causes of the poor efficiency of TMDs is their surface without "dangling" bonds which, while being advantageous for carrier mobility, causes a large contact resistance between the TMD and the metal electrode. Furthermore, a well-established procedure to control the doping of two-dimensional semiconductors is lacking, since, for example the ion bombardment method that could be in principle be used, is destructive and introduces structural defects that hinder the mobility of charge carriers.

The aim of this project is to perform a detailed characterization of heterojunctions between organic molecules and TMDs by means of photoemission spectroscopy, also time-resolved, aimed at determining the alignment of the electronic levels and the charge transfer dynamics across the interface. Doping by charge transfer from molecules is one of the possible procedures currently being studied for modifying the electronic properties of two-dimensional semiconductors. In general, direct charge transfer from the molecule to the TMD occurs only if the heterojunction is grown on an insulating substrate, whereas metallic substrates induce hybridization of orbitals and alignment of Fermi levels, which prevent effective doping . By studying different combinations of substrates, TMDs and molecular dopants, it will be possible to obtain useful knowledge to improve the development of devices for quantum technologies based on these materials. The study of the molecule/TMD heterojunctions on metallic substrates can also provide valid information not only for the doping of the TMD, but also for improving the contact efficiency between the TMD and the electrode. The experimental activities will be mainly carried out in joint University - CNR-IOM laboratories located at the Elettra synchrotron radiation source with advanced instrumentation that will allow the PhD student to carry out experimental measurements with temporal resolution by combining pulsed laser and synchrotron sources.