Strain-driven patterning of two-dimensional materials

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Transition Metal Dichalcogenides TMDs, with chemical formula MX_2, where M: metal (Mo or W) and X: chalcogen (S or Se), have received a lot of attention in the last years since they are two dimensional semiconductors with sizable band gap and particularly suitable materials for optoelectronics and optomechanics. In bulk samples, stacked X-M-X planes are coupled by van der Waals forces and the gap is usually indirect. In the single X-M-X layer form TMDs undergo an indirect-to-direct band gap transition, yielding a giant increase of the emission efficiency. For these reasons they are expected to complement graphene, for which the lack of bandgap dramatically hampers its applicability in digital electronics. Importantly, few-layer TMDs can withstand surprisingly large mechanical deformations and it is possibile to manipulate the optical and electronic properties of TMDs with the tailoring of strain. So far, most of the approaches to induce strain either require the use of external, bulky devices or rely on spontaneous, yet not controllable, mechanisms. An alternative route is to exploit the capability of layered 2D materials to deform at the micro- and nano-scale due to the presence of atomic or molecular species trapped in between adjacent layers. Specifically, proton irradiation and atom (H, He, Ar, Xe) intercalation can be used to create gas-filled TMD domes, whose thickness is just one layer. It was recently shown that low-energy proton irradiation leads to the formation of hydrogen-filled TDM domes on top of multilayer flakes, thanks to the catalytic properties of MX_2 samples that trigger the production of H_2 molecules just beneath the top layer. Therein a spatially localized partial exfoliation of the material takes place and spherically shaped domes appear with a random distribution on the sample surface. The domes so created are just one X-M-X plane thick, with a footprint diameter that can be varied , so far, from 10 μm to 50 nm, durable against aging and mechanical stress and emit light efficiently at room temperature (RT).

My PhD activity will be based on a project whose aim is to engineer a non-uniform strain at the nanoscale in TDMs. For this purpose the strain gradient can be exploited for the so called funnel effect (the possibility of controlling exciton motion by means of inhomogenous strains). This would allow an additional tunable control of the electronic properties, leading to strain-tunable optoelectronic devices. In addition, pushing the dome size at the 10 nm scale or less would allow to achieve exciton confinement to be exploited for the realization of site controlled single photon emitters working at RT. This proposal is based on a collaboration with Rome (Prof. Antonio Polimeni, La Sapienza) for the part related to proton implantation. Within this context, optical characterization achievable with advanced spectroscopy and microscopy techniques is of crucial importance. The structures will be investigated with the following methods:

- **Micro-PL** and **Scanning Near-field Optical Microscopy,** characterized by a sub-diffraction limited resolution of the order of 100 nm, will be used to study the emission properties of TMD domes arrays, and to address the nature of the fundamental optical transition as a function of strain.
- **Time resolved-PL** combined with the spatial resolution of a low temperature confocal microscope will be used to compare the excitonic lifetime determined in nano-domes with different size thus inferring important information on how carrier dynamics is affected by confinement. In order to demonstrate the RT single photon emitter nature of the smaller domes second order **autocorrelation function experiments** will be performed.