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| Project title: | **Functionalized silicene from first principles** |
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*Research project hypothesis and objectives*

The aim of the project is functionalization of silicene, i.e. changing its structural, electronic and magnetic properties by adsorption of single atoms and a combination of selected (listed below) mechanisms.

Despite its excellent transport properties (high Fermi velocity, mobility of charge carriers and the electrical conductivity), this material is not useful in electronics, where due to the need to regulate the flow of current semiconductors are used. On the other hand, silicene interactions with the environment lead to a change in its atomic and electronic structure. Breaking the symmetry between sublattices of silicene (equivalent in the case of the free layer) will lead to the creation of the energy gap around the Fermi level. In the esearch we want to prove that it is possible to control the magnitude of the energy gap by an appropriate selection of the processes affecting the structure of silicene and their parameters. We propose the use of several additional mechanisms (parameters) prior to the adsorption:

1. electron and hole doping (surface density of doped charge),
2. external electric field perpendicular to the plane of silicene (field intensity),
3. one- and two-dimensional strain.

The above mechanisms have already been studied in literature. However, they were considered separately. In the proposal we shall focus on functionalization of silicene by adsorption of single atoms of light and heavy elements in the presence of other mechanisms, like charge doping, external electric field and strain. For all cases, we shall determine the relationships between parameters that modify the structure of silicene and the magnitude of the resulting energy gap. Furthermore, the magnetic properties of silicene with adsorbed atoms as well as kinetic properties (in particular diffusion and desorption parameters) of adatoms on silicene will also be studied. We expect that exploring the relationships between different mechanisms that modify the electronic structure of silicene, we shall be able to offer the most effective method of controlling its energy gap and magnetic properties.

The second objective is to determine changes in the electronic structure of silicene in the case of structural modulation (corrugations) in the nanometer scale (several lattice constants) in one direction. This effect, albeit not strong, has been observed in the case of graphene. We expect that similar modification of silicene geometry will lead to a change in the slope of the bands around the K points of Brilloiun zone in this direction and the exact shape of the Dirac cone will depend on the geometry of the corrugation and on the magnitude of buckling. The one-dimensional structural modulation of silicene may also be regarded as one of the possible mechanisms of functionalization, in particular in connections with fabrication of silicene layers on vicinal (stepped) surfaces.