Project 6.5 Excitonic effects in perovskites for the photovoltaic and laser applications

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Background:

Perovskites ABX3 (A=methylammonium,formamidinium,Cs,Rb and B=Pb,Sn and X=Cl,Br,I), their low-dimensional structures, such as 2D, nanowires, quantum dots, and the heterostructures with organic layers continuously attract interest of researchers as photovoltaic and optoelectronic materials (LEDs, lasers and detectors). Since 2014, the optically pumped perovskite lasers, both short-pulse and continuous-wave type, were reported. However, a construction of the electrically pumped laser still remains a challenge, being one of our tasks. The excitonic binding energies in these materials range 25-400 meV, and probably this is not a record. Due to a high light-refractive index (of 2.2-2.5) at the perovskite-air interface, natural nanostructure cavities do not require mirrors. Moreover, an integrated system with the perovskite optically-active layer and topological edge-state mirrors could be achieved, with application to polariton lasers.

Accurate calculation of the interesting properties is possible within the framework of the Green functions formalism, from the Bethe-Salpeter equation (Yambo code), using the eigenvalues and eigenvectors of the mean-field Hamiltonian from the DFT (Quantum-Espresso code) as an input for the construction of the non-interacting Green function and the self-energy operator.

Aim:

The aim of this project is to become skillful in using the computer tools for excitonic properties of materials, and to understand the mechanisms of strong (for lasers) and weak (for solar cells) paring of the electron and hole. These mechanisms should be correlated with the corresponding geometric and chemical structures of perovskites. The electrically-pumped perovskite laser will be theoretically proposed and should be built in the experimental groups which collaborate with us.

Requirements:

- the candidate should possess a master degree obtained in one of the faculties: physics, chemistry, computer science or similar. He/she should be strongly motivated for research in the computation materials science, and be prepared to work with the linux environment,
- knowledge of English language is very useful,
- we invite the candidates with the knowledge of at least one language of the computer programming.