

Master and Engineer Internship: 2019-2020

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Title: Modeling of electronic structures of self assembled molecular layers on

Germanium

Abstract:

The main objectives would undertake the theoretical investigation of thiol based push-pull molecules grafted on Germanium. The first task would to build the molecules and investigate their electronic properties. Next, probably a key scientific roadblock is probably the grafting of thiol based molecules on germanium will be investigated and model of possible grafting proposed. Finally, the main objectives would to simulate the electronic transport in these heterojunctions made by the self-assembled monolayers, the contact with the germanium surface and local electrical probes.

For this intership, an experience in chemical and materials modeling would be necessary and also in numerical modeling (octave, script)...











