Study of DFTB modeling for strongly charged systems

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This training period is proposed in the context of the atom probe tomography (APT). The successful candidate will train alongside a beginning PhD student working on the same subject.

The APT is a unique material analysis tool allowing to get the chemical composition of solids, both qualitatively and in three dimensions. Basically the process is the following: a sharp tip is trimmed from the bulk material; cooled; placed in a vacuum chamber; submitted to a high potential difference with respect to a position sensitive detector; submitted to pulsed laser irradiation; evaporated. This process allows to determine the initial position on the tip of each atom thanks to the detector, and numerical analysis. The numerical process being used to determine the complete trajectory of each fragment from the tip to the detector.

Unfortunately for some compounds the process is not that simple: some fragments may not be detected, the computed trajectory are not as accurate as one may wish. For some materials the modeling is accurate enough, for others it is not. Our team is working on improving the knowledge about the very beginning of trajectories for $Al_xGa_{1-x}N$ compounds.

In order to improve the modeling of the ejection process of fragments out of the tip — a major source of modeling error in current APT experiments — we are developing a

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DFTB analysis tool.

DFTB (density-functional tight-binding[1]) seems indeed a good candidate to improve the knowledge of the processes at the edge of the tip. It allows to get a sensible description of the electronic structure of material samples big enough to model the tip. It also has already been used for the study of other charged systems (eg : for instance in simulating electrodes[2]).

We are aiming at pushing the DFTB modeling further. For the APT we must be able to study multiply charged fragment. This require new parameters for DFTB, and new algorithms to solve DFTB problems.

Work: Depending on the current status of our project and his own interest the trainee's work may be twofold. On one side stand some classical electronic structure calculations (using density functional theory (DFTB) or post-Hartree-Fock methods) and multi-parameters optimisations for the DFTB model fitting. On the other side abide works on the core algorithms of DFTB to allow performing the kind of computation we need. For instance the training period could be devoted to performing electronic structure computation on Gallium — parallel to a study already performed on Aluminium — in order to get a sensible parametrisation of Gallium properties in DFTB. Every way, the work will help and require to develop skills in computer uses and programming.

[1] M. Elstner *et al.,* Self-consistent-charge density-functional tight-binding method for simulations of complex materials properties, Physical review B, volume 28, number 11, p. 7260

[2] DFTB modeling of lithium intercalated graphite with machine-learned repulsive potential. arXiv: 1904.13352