Simulation en DFTB d'agrégats chargés à l'aide de charges obtenues par méthode de machine-learning

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Abstract
Atom Probe Tomograpgy (APT) is an experimental metrology tool intended to explore atomic arrangement in solids. Its working principle is field emission used to evaporate atoms from the sample surface, which is given a needle shape. The simulation work presented in this thesis takes place in the APT framework and is dedicated to better understanding of field emission. We focus on silicon carbide (SiC) as a typical semiconductor often studied in APT. To perform a relevant simulation, in is necessary to consider a large number of atoms while keeping the physico-chemical specificities of the material at a good level of description. To reach our goal, we have developed a machine learning method based on tight binding density functional called ML-DFTB. It is sufficiently accurate to describe the electronic structure of the material in a quantum chemical framework while being computationally efficient. The addition of machine learning to DFT provides us a mean to get the atomic charge in an a priori approach. When combined with a redefinition of the DFTB energy, this allows us to solve efficiently the numerical problem, by bypassing the self-consistent iterative search for atomic charges of the SCC-DFTB method. We validate our approach by means of systematic comparison of ML-DFTB calculations with reference calculations for small SiC clusters.