Density-Functional Calculation of Stanene

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total points: 20

In the past fifteen years, the discovery of topological insulators has revolutionized the conventional viewpoint of the states of matter. In addition to metal, semiconductor and insulator classified in solid-state physics by their unique electronic structures, topological insulators demonstrate a completely different picture, whose bulk behave like a normal semiconductor/insulator with well defined gap. However, on their surface/edges there exists nondissipative charge/spin current, making the topological insulator a new state of matter that cannot be understood by conventional band theory.

It now becomes clear that the unique nature of the topological insulators is deeply related to their nontrivial berry curvature which, for a long time, has been believed to be unimportant. There exists many materials demonstrating certain level of topological properties. In this exercise, you will examine one simple yet very interesting topological insulator, *i.e.* stanene - a monolayer Sn atoms with honeycomb structure.

Please carefully read "Large-Gap Quantum Spin Hall Insulators in Tin Films" by Yong Xu et al, at Phys. Rev. Lett. **111**, 136804 (2013) and try to repeat figure 2 and figure 3. To be more specific, you are about to do

1. Construct the crystal model for stanene, You can refer to figure 1c for the lattice constants and relax the internal coordinates of Sn atoms automatically with DFT. Similar to the first example discussed during the lecture (`https://cms.mpi.univie.ac.at/wiki/index.php/Fcc_Si`), to get the lattice constant precisely, you need to try different values of the lattice constant and look for the one with the lowest energy.

2. Calculate the bulk electronic structure for the three cases shown in figure 2(a-c). Note that, for each case, one needs to first get the corresponding relaxed structure based on which the electronic structure is calculated.

3. Construct slab geometry for stanene, fluorinated stanene and stanane, and calculate their edge states as shown in figure 3 (a-c).

Note that, the slab calculations (figure 3) takes long time to finish, please start your job as early as possible.