

# MOLECULAR DYNAMICS

This exercise is intended to illustrate a Molecular Dynamics run with SIESTA. The system is a Si(001) surface, in the 2x1 reconstruction with asymmetric dimers. The simulation cell contains two dimers. An H<sub>2</sub> molecule approaches the surface, above one of the dimers, and dissociates, ending up with a H atom bonded to each of the Si atoms in the dimer (and thus leading to a symmetric dimer).

First, read the input file, and pay particular attention to the variables related to the Molecular Dynamics options. Try to understand the variables, using the SIESTA user guide (at <http://www.uam.es/siesta>).

[Note that the atomic masses of the H atoms are set to those of Deuterium, instead of Hydrogen, so that larger time steps can be used.]

In order to give an initial velocity to the molecule towards the surface, you can use the MD.UseSaveXV variable in the input file, so that the initial velocities are read from the Si001+H2.XV file. An appropriate file is provided. Note that both H atoms are given an initial velocity of 0.2 bohr/fs towards the surface.

**IMPORTANT:** before each new run, you must copy the files Si001+H2.XV and Si001+H2.VERLET\_RESTART from the FILES directory. These files are needed to provide the initial velocity to the MD runs.

Run the program, and check the results. You can visualize the dynamics using the Molekel program, reading the Si001+H2.ANI file (multiple structure xyz format), or the Xcrysden program, if you convert the information in the MD file to the appropriate AXSF format using the md2axsf program by Andrei Postnikov (in Util/Contrib/APostnikov).

You can obtain extra information about the dynamics by looking at the output file, and also the file Si001+H2.MDE. In that file, the fourth column (E\_tot) shows the evolution of the total energy with time. This should be a conserved quantity in a microcanonical MD run. Why is it not in this run? What are the input variables responsible for this? Change these variables to do a standard microcanonical run, and see the result by running the code again.