A force field investigation of the influence of the metal on the breathing behaviour of MIL-53 type materials

L. Vanduyfhuys, T. Verstraelen, D. Vanpoucke, M. Waroquier, V. Van Speybroeck

Center for Molecular Modeling, Ghent University, Ghent, Belgium

Mil-53 type materials are known to have a flexible framework allowing them to undergo structural transitions with large variations of the cell volume. Breathing is an example of such a structural transition, in which the unit cell can transform from a large pore to a narrow pore under the influence of external stimuli such as temperature, pressure, gas adsorption, ... There are several reports in literature that show that the thresshold to induce breathing varies with the metal kind in Mil-53. In this work, we develop force fields for Mil-53(Al, Ga, In, Cr) using a new progam QuickFF, which is developed to quickly generate accurate valence force fields for isolated molecules from ab initio training data. The charges were derived using the new Hirshfeld-E scheme and the van der Waals interactions were taken from the MM3 force field. We then use the force fields to compare the flexibility of the various types of Mil-53. Cell parameters of large and narrow pore are compared as well as the internal energy profile of a trajectory that mimics breathing.