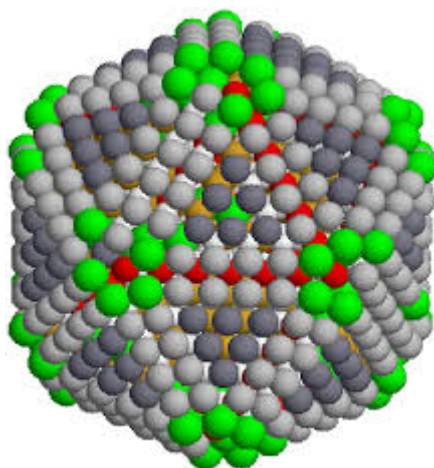


Optimization for molecular clusters

This thesis concerns the development of specific tools for the optimization of atomic clusters based on the identification of surface atoms and their relocation. No previous knowledge of chemistry is required.

The thesis will require python modules to be developed, using parallel and distributed computing



Image

credits: http://www.phys.canterbury.ac.nz/research/nano/md_shan.shtml