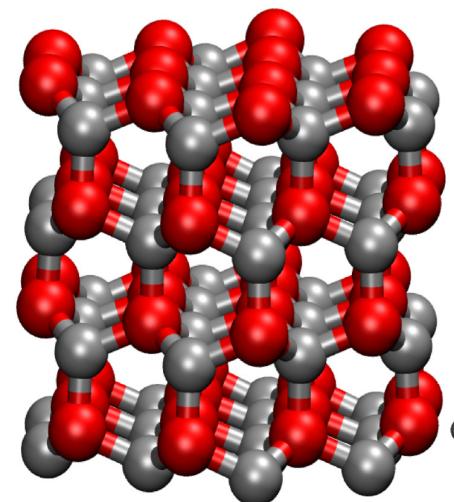


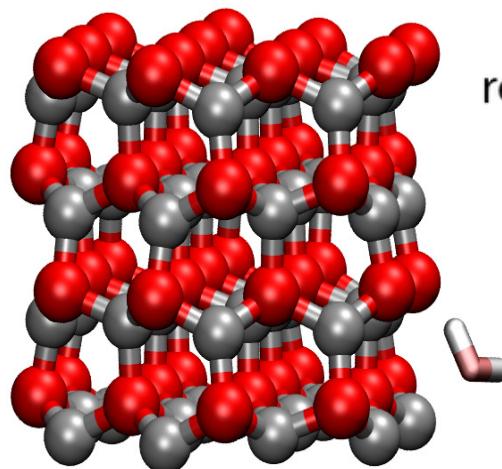
QE



1^{er}
relajación



LAMMPS



2^{da}
relajación



dftb+

