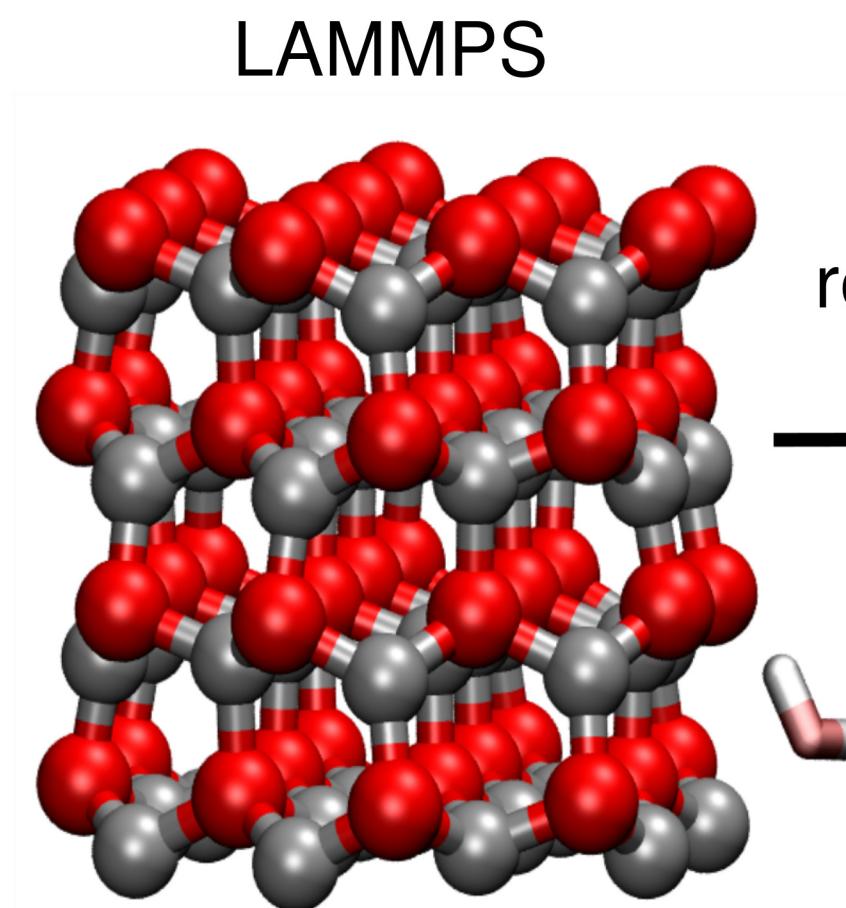


1<sup>er</sup>  
relajación

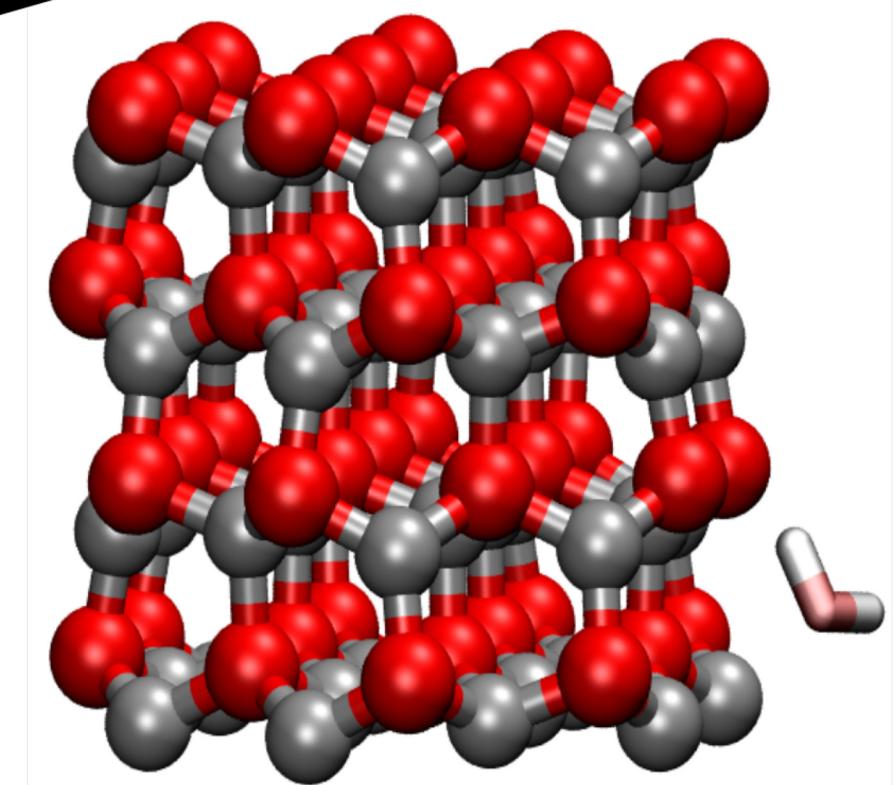
$C_A$

$C_B$



LAMMPS

2<sup>da</sup>  
relajación



dftb+



QE