Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials:

Oxygen Vacancy and Hole Conduction in Amorphous TiO_2

Hieu H. Pham and Lin-Wang Wang

Potentials energy of the TiO_2 system during the MD simulations (melt-and-quench process)

The common melt-and-quench technique was employed to produce the amorphous model of TiO_2. The heating and cooling processes were computationally conducted with a temperature increasing/decreasing small step of 200K. At each temperature step (during the heating, as well as the cooling), the sample is equilibrated for 100 ps using the NPT ensemble. The final amorphous structure obtained from the MD simulation was further relaxed by first-principles calculations. The plots of potential energy and temperature as a function of time, therefore, are stepwise.

The graphs below present the potential energy and temperature as a function of time.

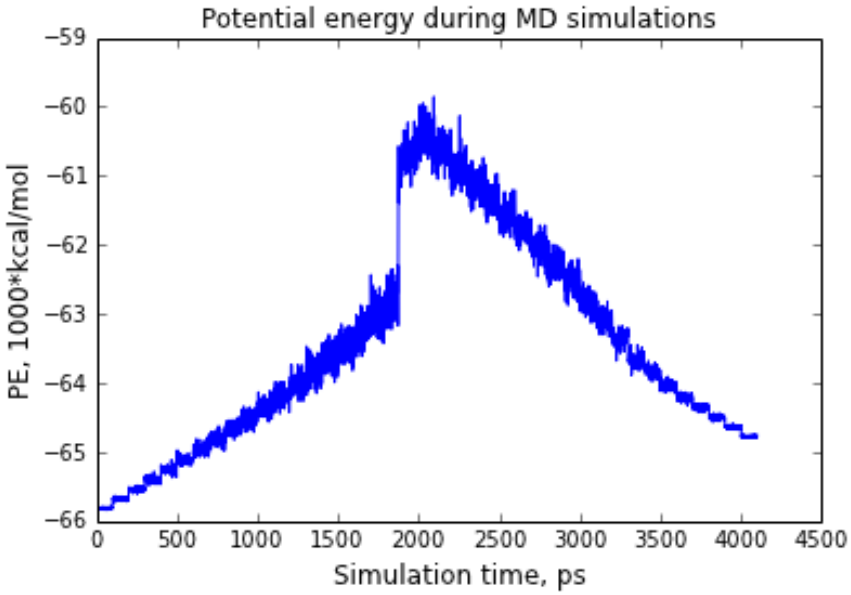

Figure 1. Potential energy as a function of simulation time (ps). The sudden jump in the graph (at 1800 ps) corresponds to the transformation from the crystalline structure (this graph was shown for rutile) to the amorphous phase (melting)

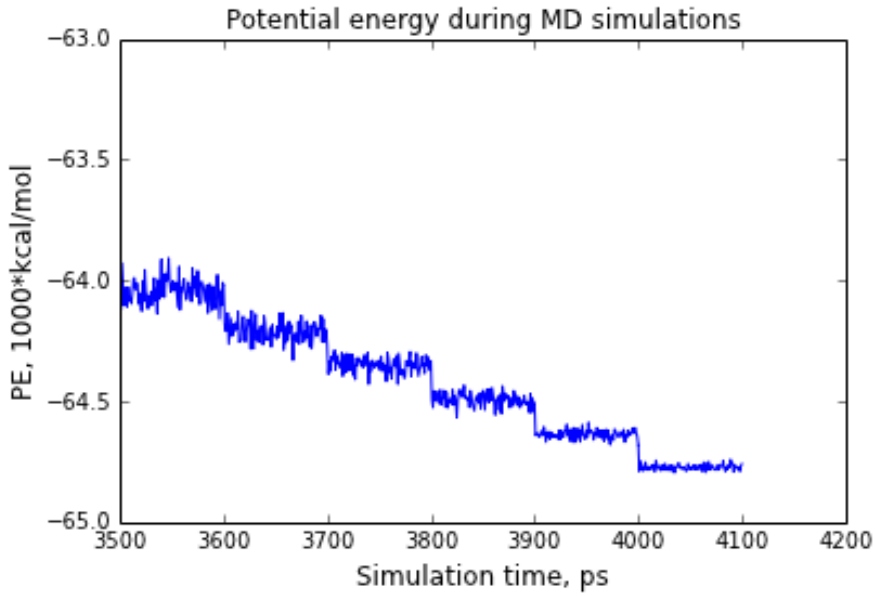

Figure 2. Potential energy shown for last steps of the cooling process

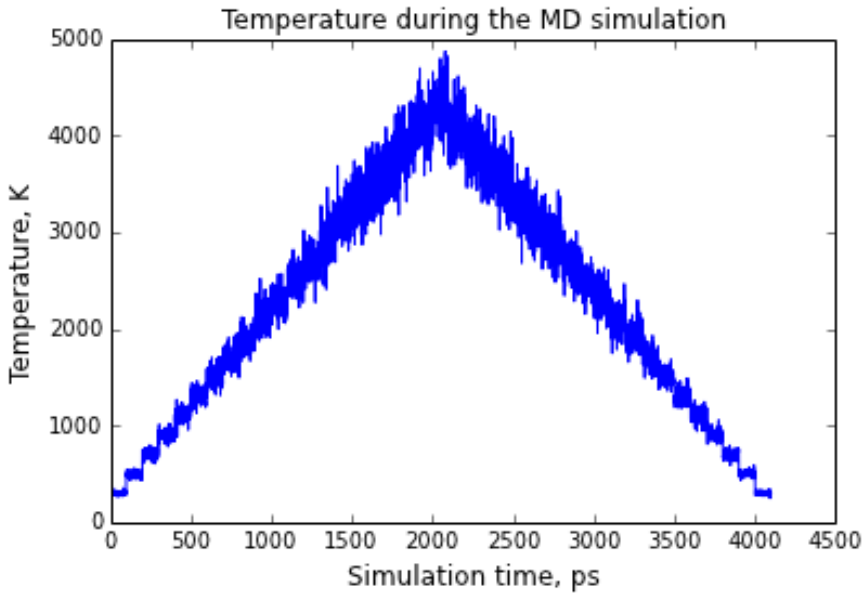

Figure 3. Temperature as a function of simulation time (ps)

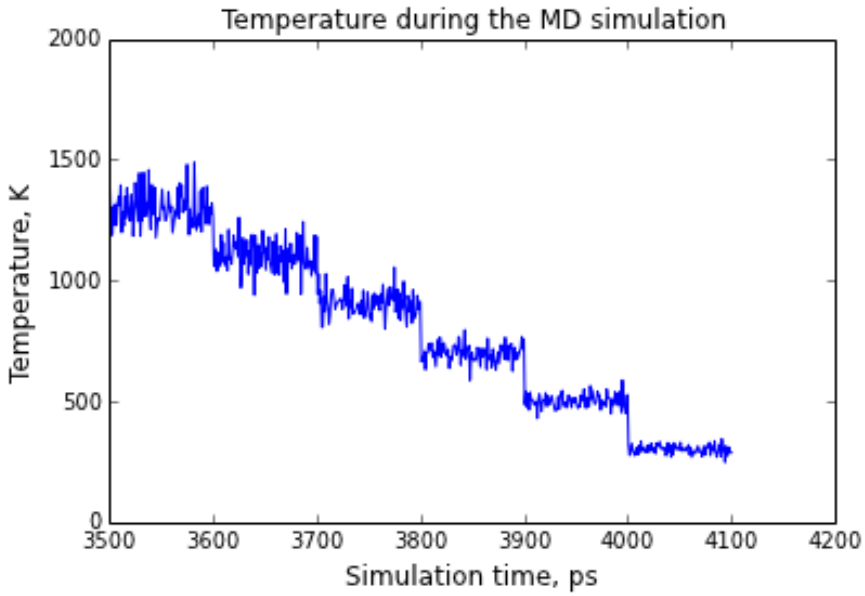

Figure 4. Temperature as a function of time (ps), during the last steps of the cooling process

The radial distribution function of TiO2 system during the MD simulations

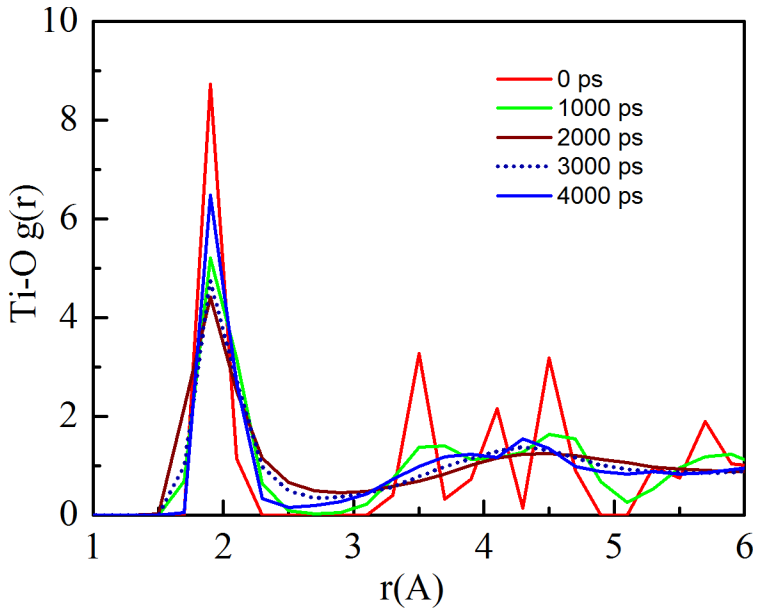

Figure 5. The radial distribution functions of the Ti-O pair at different time during the MD simulation. The nearest neighbor Ti-O bond distance stays the same as a function of time.

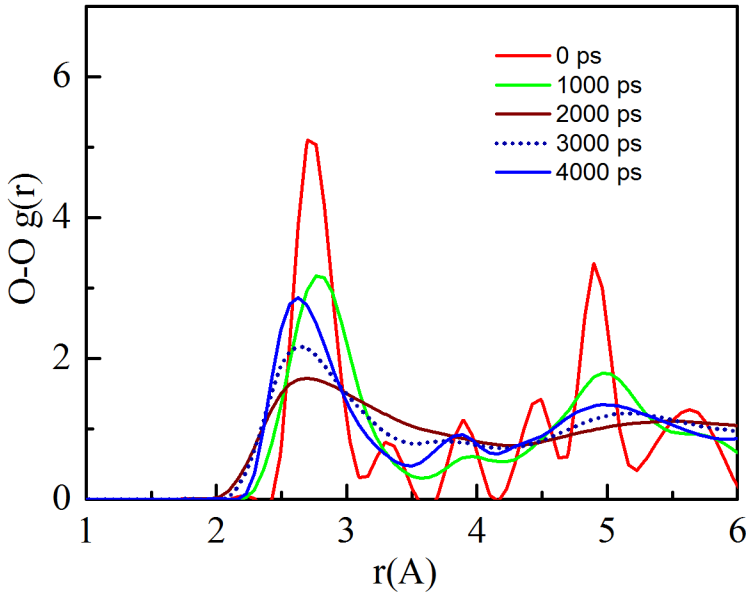

Figure 6. The radial distribution functions of the O-O pair at different time during the MD simulation

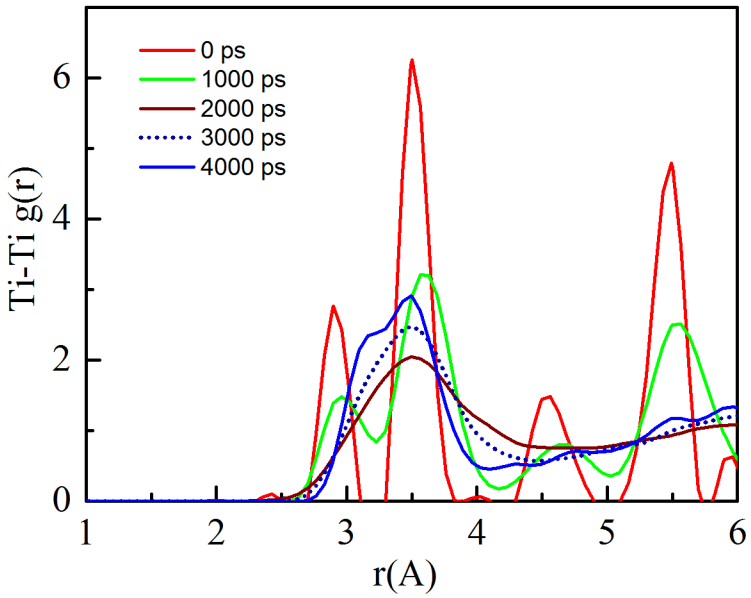

Figure 7. The radial distribution functions of the Ti-Ti pair at different time during the MD simulation