Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Thermal Stability of Aluminum Oxide Nanoparticles: Role of Oxygen Concentration

Supplementary Material

Melting points

Melting point is calculated from volume per atom vs temperature curves, the transition in both curves correspond to the material melting point.

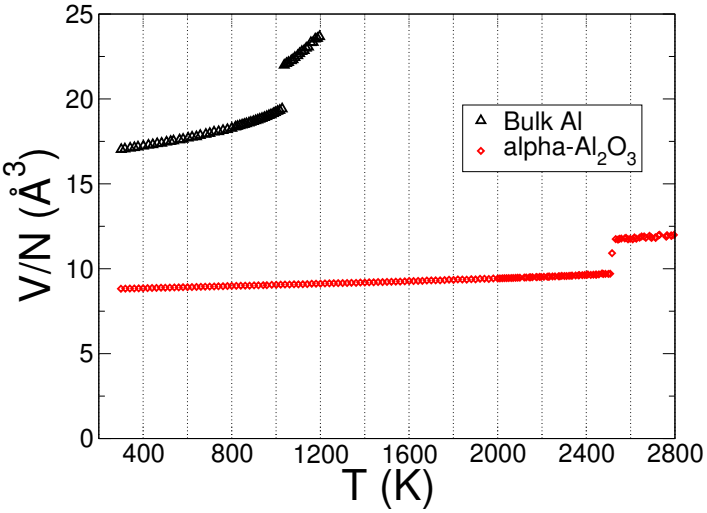

Fig. 1 Volume per atom versus temperature curves, for Al and α-Al_2O_3 bulks.

Statistical distribution

Energy histogram of 2000 seeds used for MonteCarlo Algorithm, for a $Al_{147}O_{30}$.

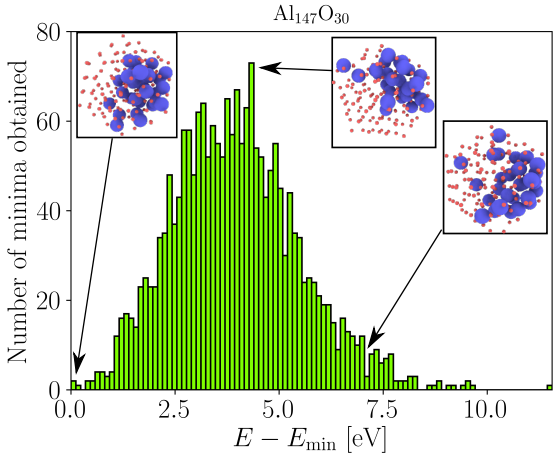

Fig. 2 Energy histogram of a $Al_{147}O_{30}$, three representative structures are depicted in the figure inset

DFT calculations

The Fig.3 show a comparison between DFT and MD calculations. Initial structures correspond to MD obtained NP with ReaxFF. Final structure use ReaxFF as a seed for DFT calculations

Based on the histogram of interatomic distances, between Al and specific elements (Al or O), before and after the atomic relaxation, we can see slightly shortened distances. These variations do not show any significant structural change, therefore the initial configurations obtained by MD simulations are located close to local minima at DFT level.

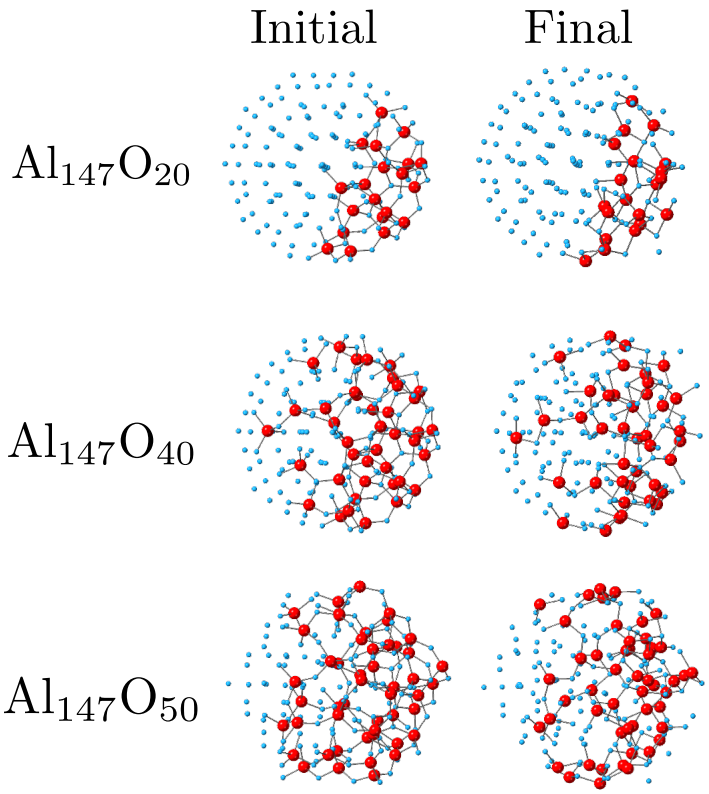

Fig. 3 Clusters of $Al_{147}O_{20}$, $Al_{147}O_{40}$ and $Al_{147}O_{50}$ after a energy minimization. Initial configurations are considered from MD simulations. Light blue and red atoms correspond to O and Al atoms respectively.

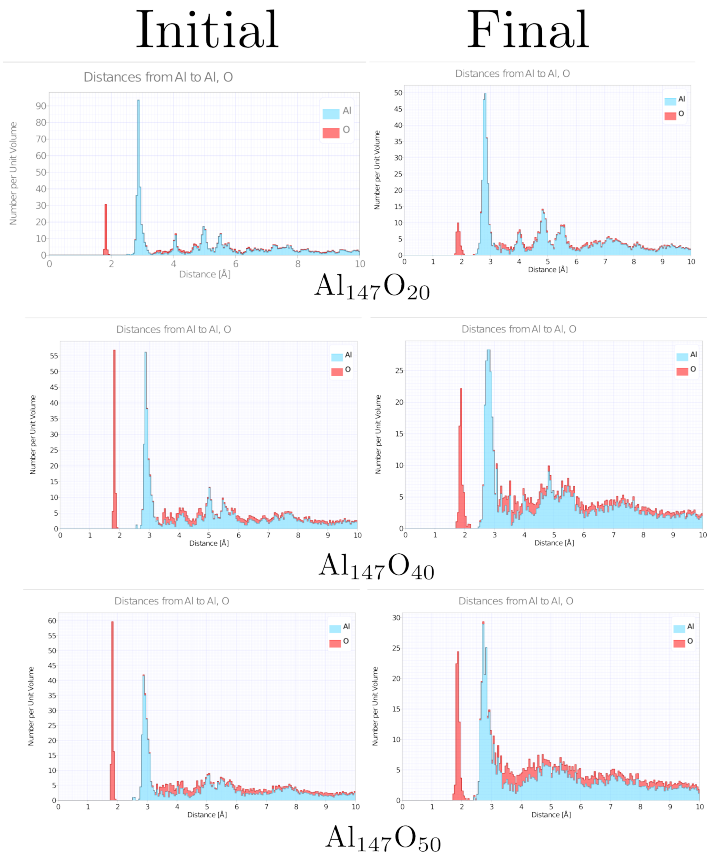

Fig. 4 Bonds length for $Al_{147}O_{20}$, $Al_{147}O_{40}$ and $Al_{147}O_{50}$ after a energy minimization. Initial configurations its taken after a previos MD simulations.