Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Structure, intermolecular interactions, and dynamic properties of NTO crystal with impurity defects: A computational study

Jincheng Ji, Kun Wang, Simin, Zhu and Weihua Zhu*

Institute for Computation in Molecular and Materials Science, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094,

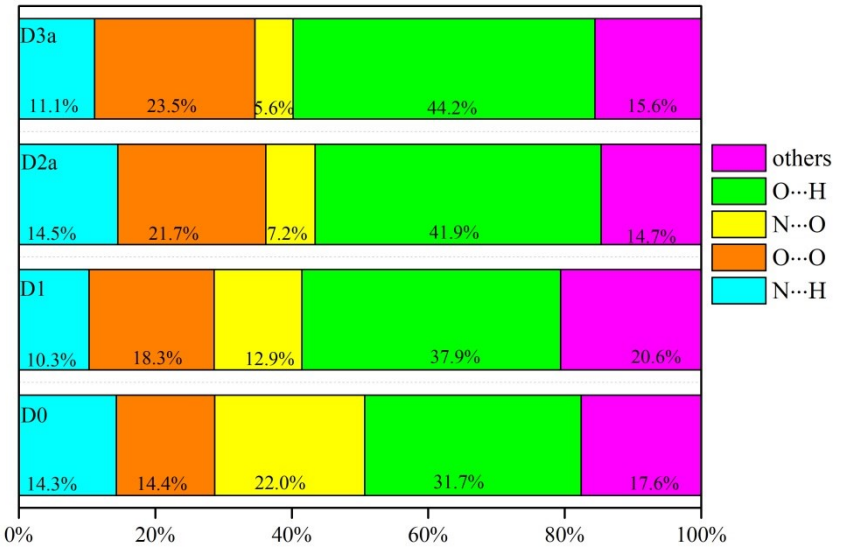

Fig. S1 Contact distribution of the NTO molecules in the ideal and impurity-contained NTO crystals.

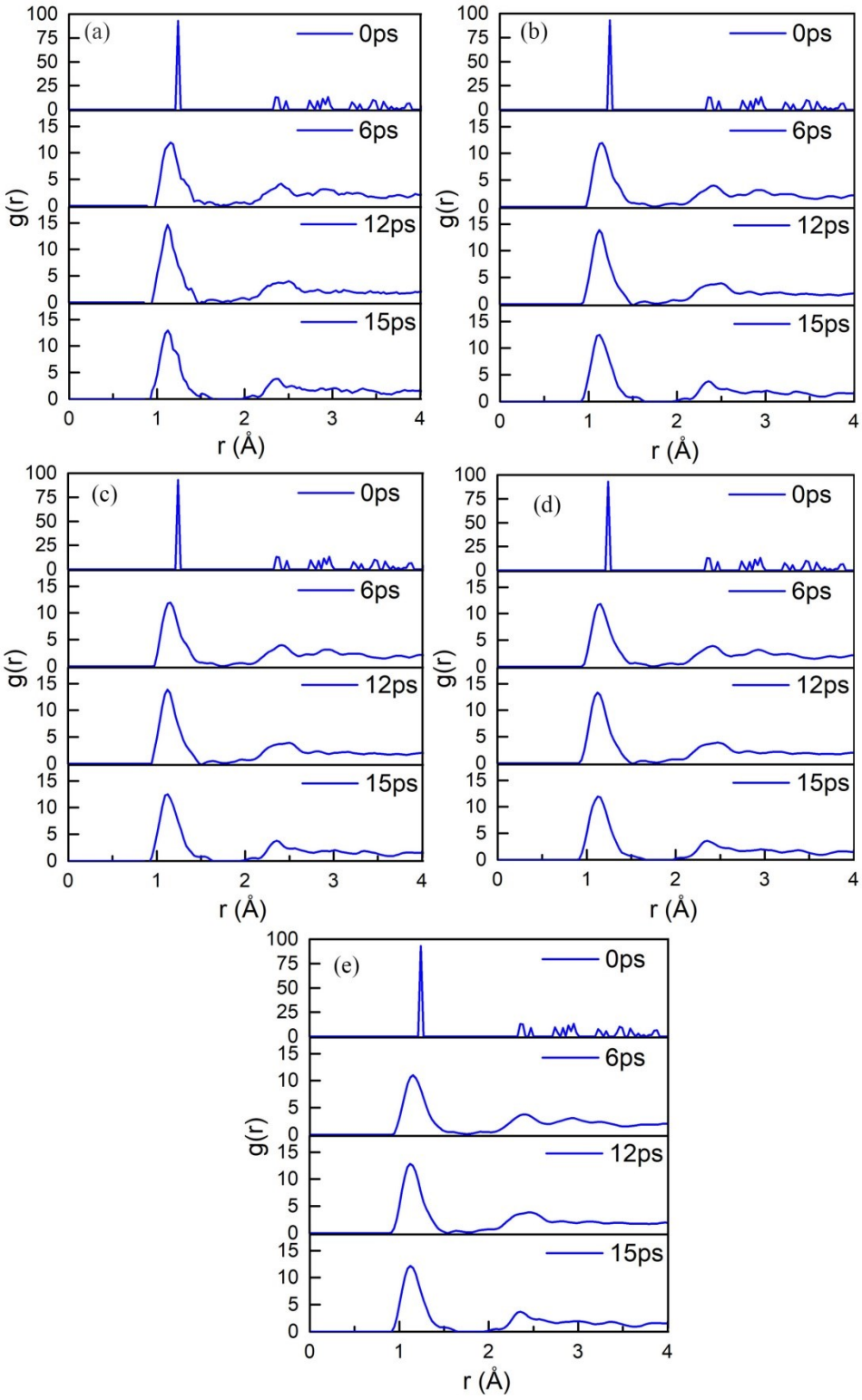

Fig. S2 The RDFs of the D0 model from the five MD simulations