Supporting Information

Ab-initio Study of Sodium Insertion in the λ-Mn_2O_4 and dis/ordered λ-$Mn_{1.5}Ni_{0.5}O_4$ Spinels

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A.

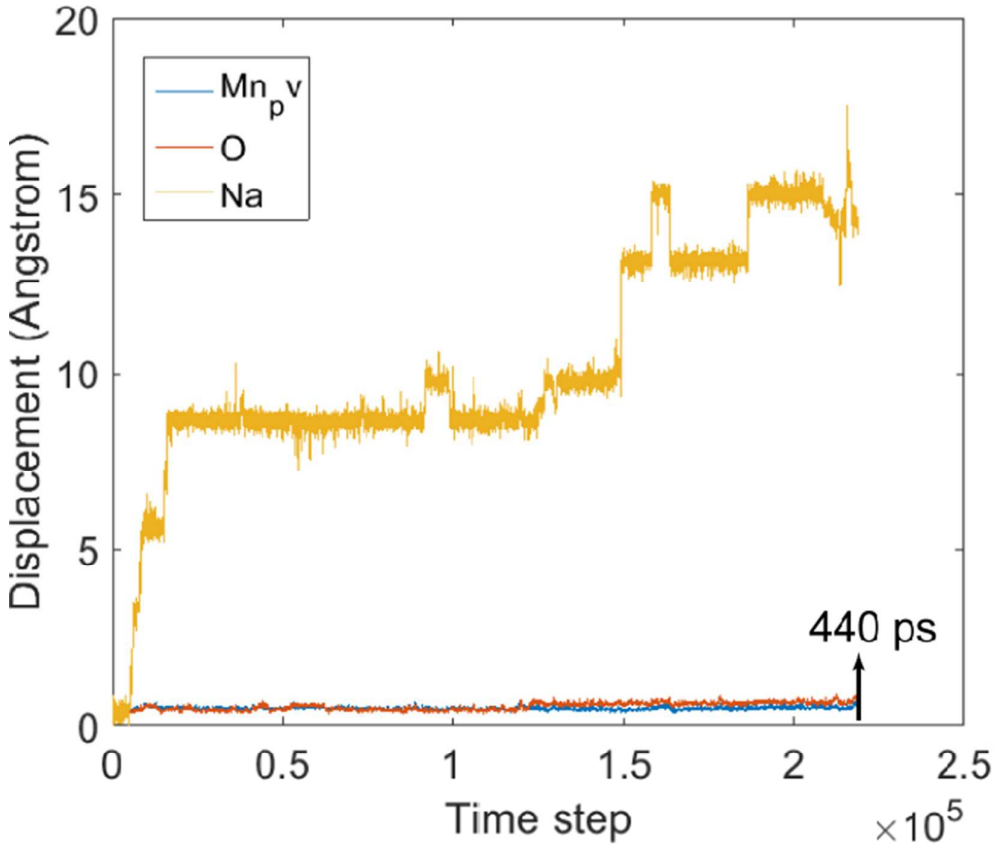

Figure S1: Atom displacements for a 440 ps MD simulation of the pure spinel phase at 600 K

B.

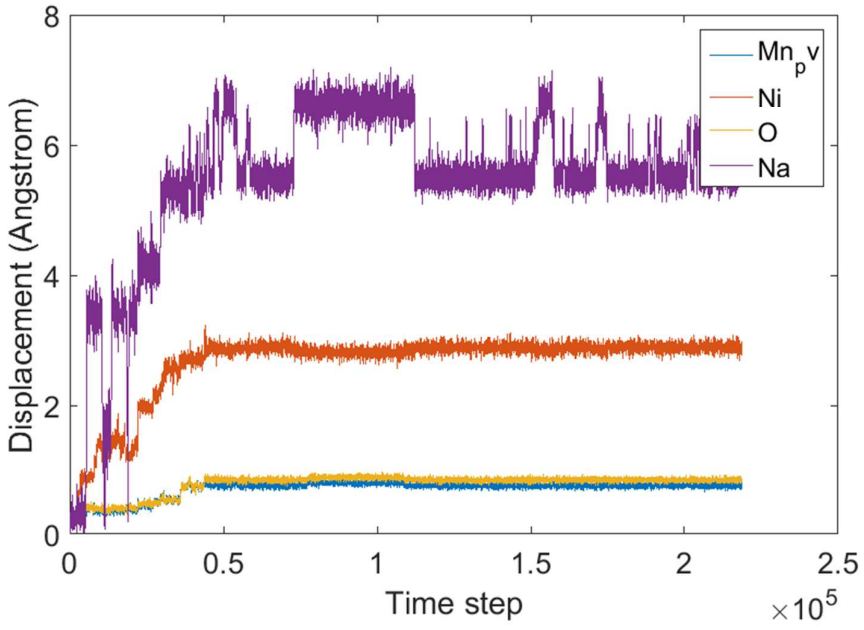

Figure S2: Atom displacements for a 440 ps MD simulation of the F2- MNO phase at 600 K

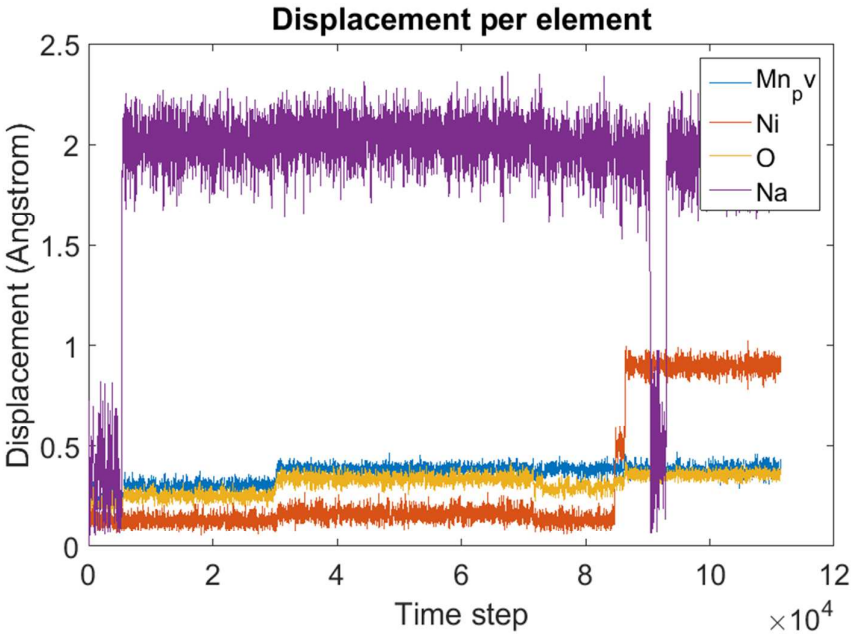

Figure S3: Atom displacements for a 240 ps MD simulation of the F2- MNO phase at 300 K

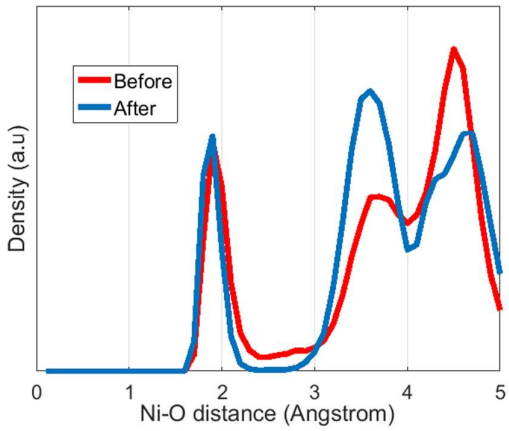

Figure S4: Ni - O radial distribution function (RDF) for one of the nickel atoms before and after it moves to the new position

C

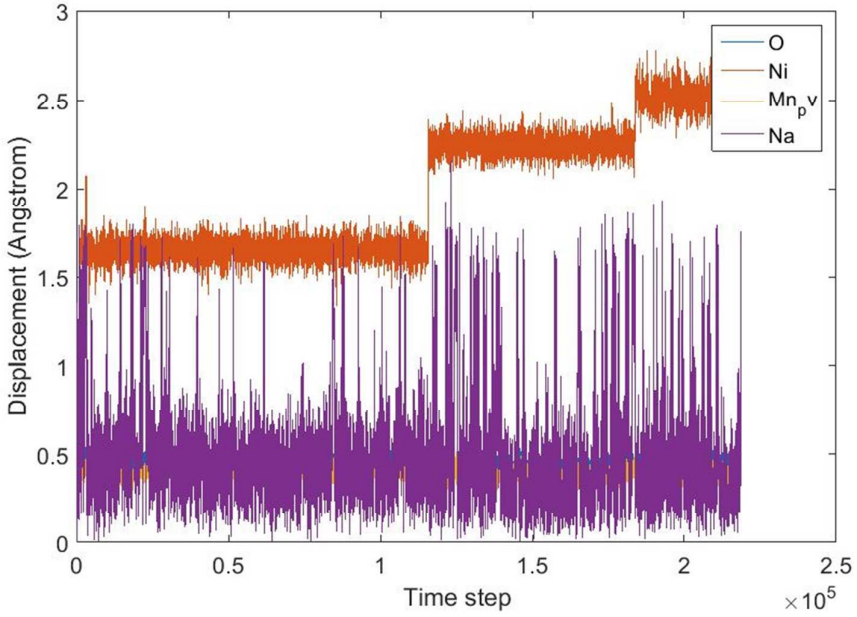

Figure S5: Atom displacements for a 440 ps MD simulation of the P- MNO phase at 600 K

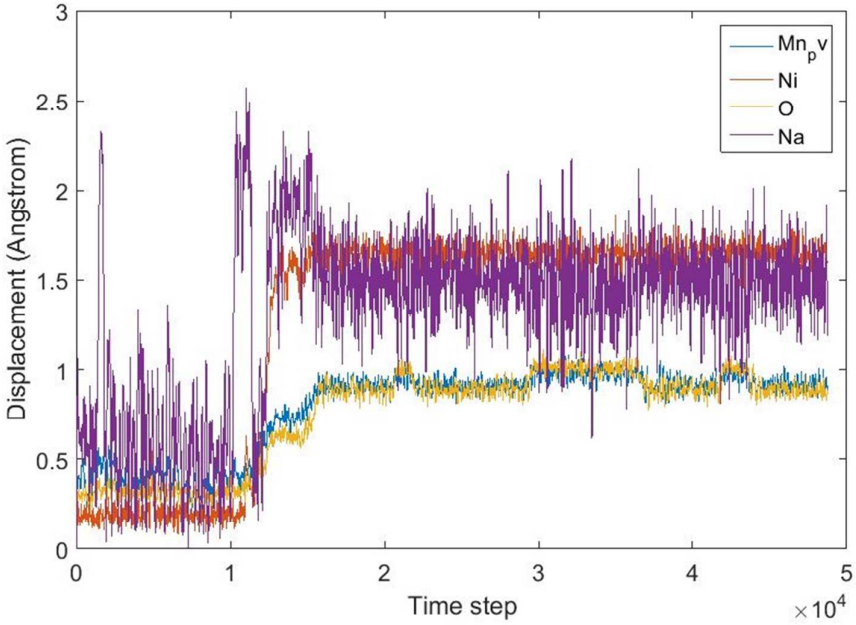

Figure S6: Atom displacements for a 100 ps MD simulation of the F1- MNO phase at 600 K