Supplementary information for "Predicting Electrochemical Properties and Ionic Diffusion in $Na_{2+2x}Mn_{2-x}(SO_4)_3$: Crafting a Promising High Voltage Cathode Material"

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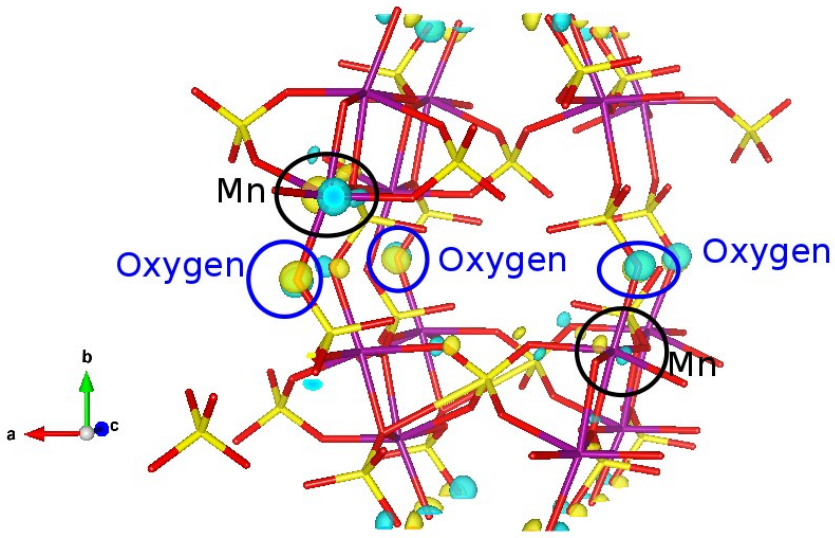

Figure 01: Charge-density difference ($\Delta\rho(r)=\rho(Na_{2.5}Mn_{1.75}(SO_4)_3)$ $\rho(Na_{2.5}Mn_{1.75}(SO_4)_3\_defective)+ \rho(Na)))$ where ρ is the charge-density of a Na placed in one of the Na2 positions. Blue and yellow are the isosurfaces at +-0.09 e^- per $Å^3$.

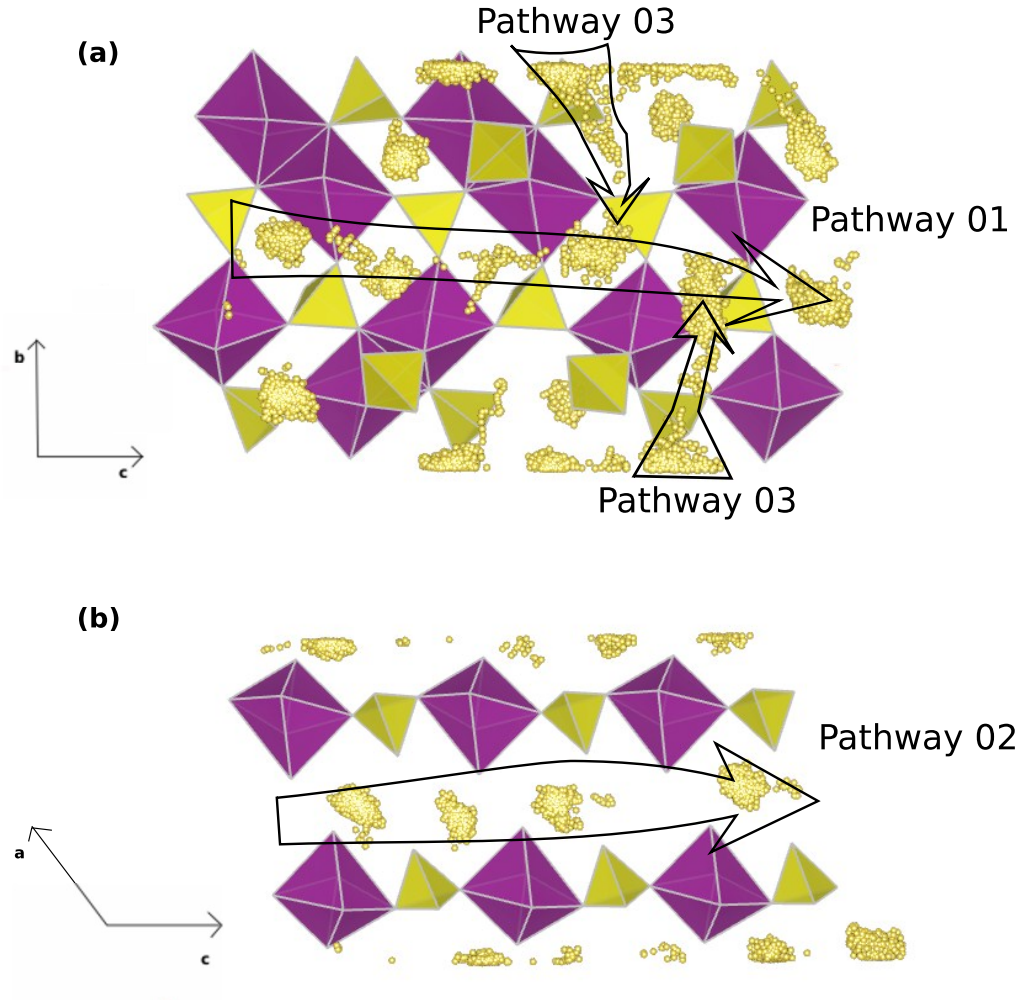

Figure 02: (a) Snap shots of the IAMD showed in the bc plane of the $Na_{2.5}Mn_{1.75}(SO_4)_3$ crystal structure. (a) The arrows indicate the possible diffusion pathways followed by Na ions. In this case, pathway 01 and pathway 03 are highlighted. (b) Snapshots of the IAMD showed in the ac plane of the $Na_{2.5}Mn_{1.75}(SO_4)_3$ crystal structure. The arrow indicates the possible diffusion process occurring in the [001] direction by hopping through Na3 to Na3 atoms.

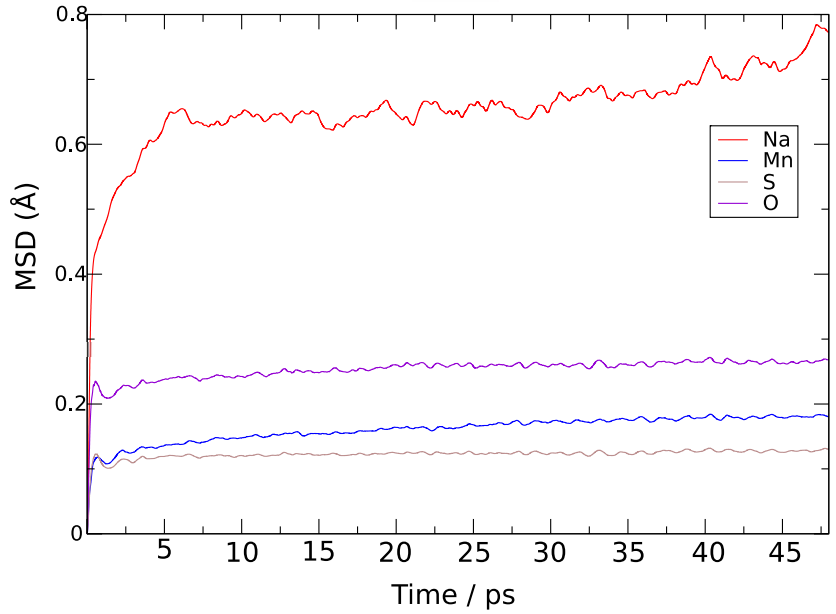

Figure 03: Mean-squared displacement (MSD) of Na, Mn, S and O atoms at 600 K.

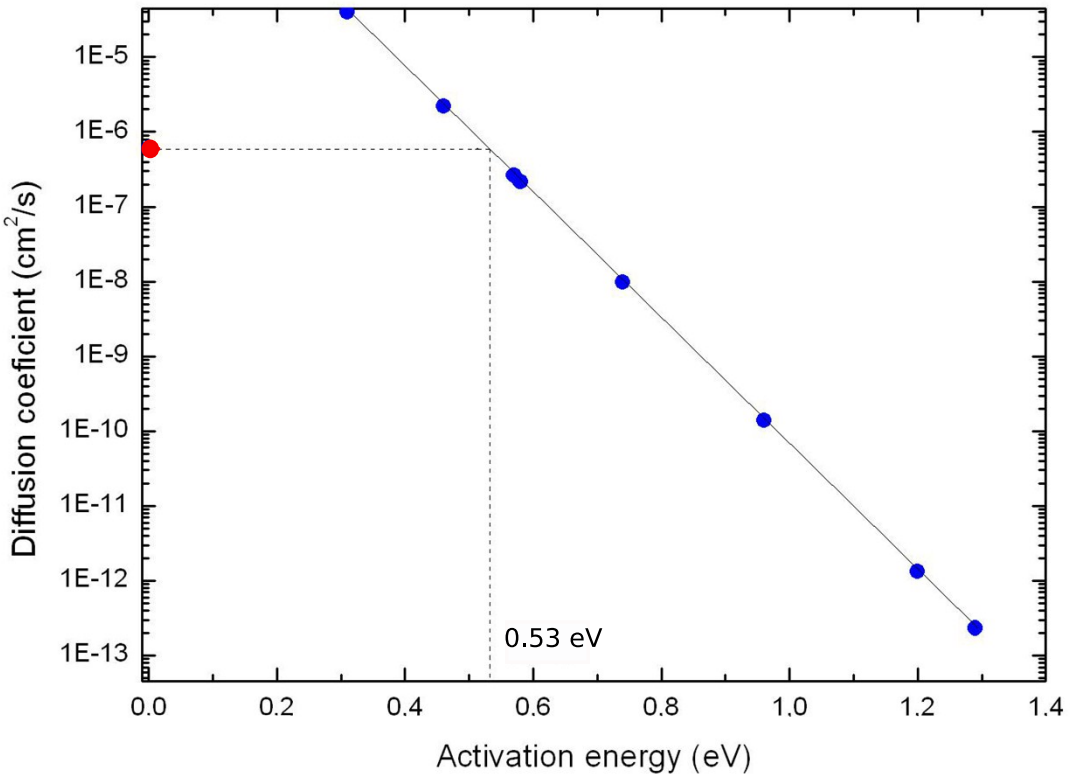

Figure 04: Blue line represents the diffusion coefficient calculated as $D=d^2\Gamma$ for the activation energies of Tab. 03. Here, d is the average hop distance, Γ is defined as $\Gamma = v_0 exp\left(-\frac{E_a}{k_b T}\right)$, with v_0 being the attempt frequency, E_a as the activation energy, k_b the Bolzmann constant and T the temperature (in this case 600 K). The red ball is the diffusion computed through the MSD of the molecular dynamics calculation. The dashed line is the extrapolation for the activation energy that better represent the diffusion coefficient from the MD. In this case this value assumes 0.53 eV.