SUPPLEMENTARY INFORMATION

Hybrid Functional Study on Small Polaron Formation and Ion Diffusion in the Cathode material Na$_2$Mn$_3$(SO$_4$)$_4$

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Figure S1: Magnetic moment alignment of Mn ions in configurations AFM1 (a), AFM2 (b), AFM4 (c) and AFM4 (d). Red and blue arrows denote the up and down directions.

Figure S2: DOS of the vacancy structure Na$_3$[Mn$_3$(SO$_4$)$_4$]$_4$ by GGA+U (U=3.9 eV). Fermi level is set at 0.0 eV.