**Supporting Information** 

## Unveiling the thermodynamic and kinetic properties of Eldfellite, NaFe(SO<sub>4</sub>)<sub>2</sub>: toward a high-capacity and low-cost cathode material

Amitava Banerjee\*a, Rafael B. Araujo\*a and Rajeev Ahujaa,b

<sup>a</sup>Condensed Matter Theory Group, Department of Physics and Astronomy, Box 516, Uppsala University, S-75120 Uppsala, Sweden.

<sup>&</sup>lt;sup>b</sup>Applied Materials Physics, Department of Materials and Engineering, Royal Institute of Technology (KTH), S-100 44 Stockholm, Sweden.

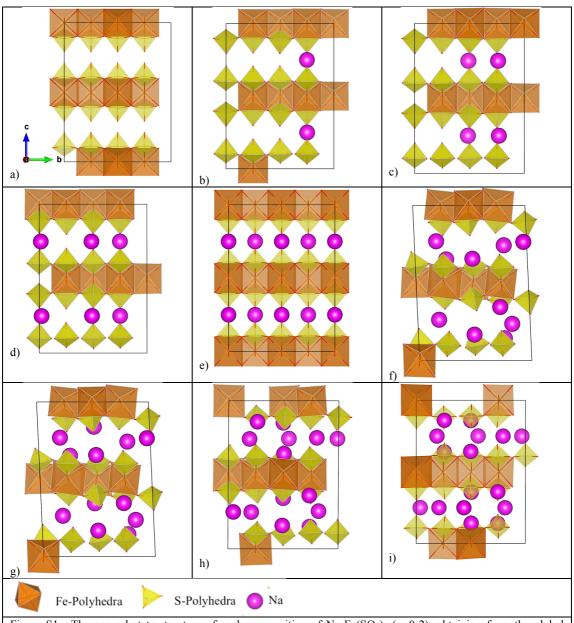


Figure S1. The ground state structure of each composition of  $Na_xFe(SO_4)_2$  (x=0-2), obtaining from the global optimization process is shown here. a)  $Na_0Fe(SO_4)_2$ , b)  $Na_{0.25}Fe(SO_4)_2$ , c)  $Na_{0.5}Fe(SO_4)_2$ , d)  $Na_{0.75}Fe(SO_4)_2$ , e)  $Na_1Fe(SO_4)_2$ , f)  $Na_{1.25}Fe(SO_4)_2$ , g)  $Na_{1.5}Fe(SO_4)_2$ , h)  $Na_{1.75}Fe(SO_4)_2$ , and i)  $Na_2Fe(SO_4)_2$ .