# Electronic Supplementary Information

# Polymorphs of $LiFeSO_4F$ as Cathode Materials for Lithium Ion Battery – A First Principle Computational Study

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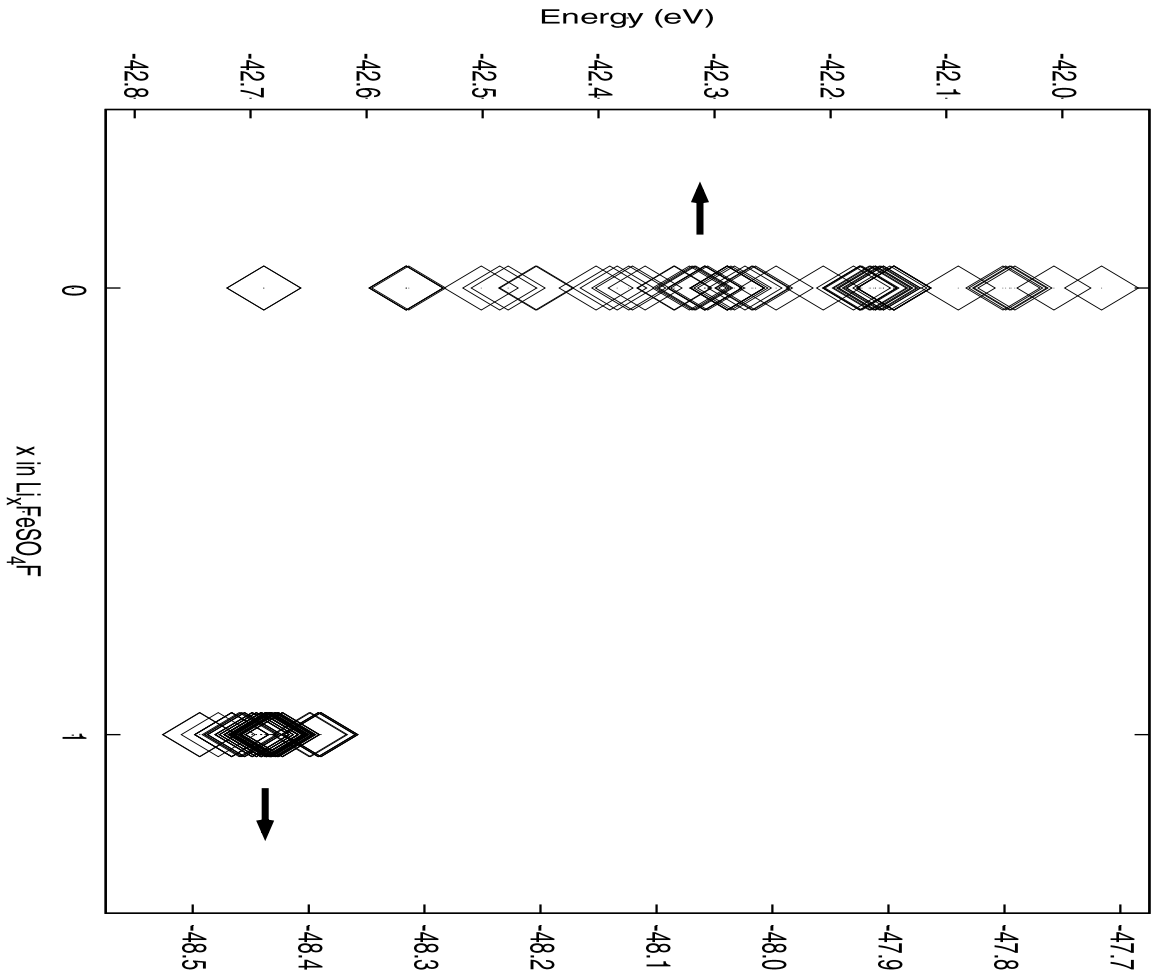


**Figure S1** Energies of the ordered structures for the triplite phase of $Li_xFeSO_4F$ (x=0, 1). There are 70 possible configurations for the permutations of the Fe/Li(vacancy) occupations. Note that the scales for the left and right ordinates are the same.

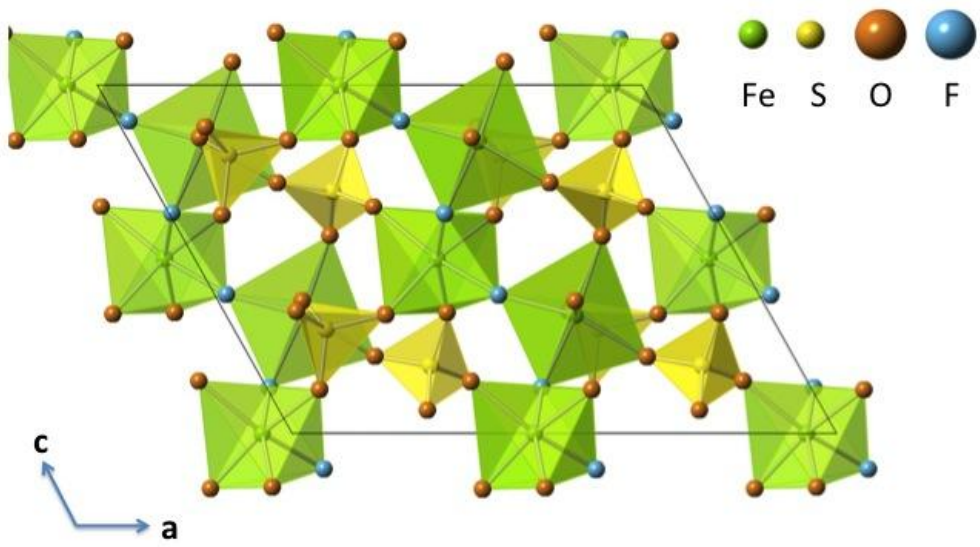


**Figure S2** Optimized structure of the triplite phase of $FeSO_4F$. This structure corresponds to the lowest energy point for x=0 in **Figure S1**.