Electronic Supplementary Material (ESI) for RSC Advances.

Supplemental Information for Article Titled: "First-principles study of structural stability, dynamical and mechanical properties of Li_2FeSiO_4 polymorphs"

P. Vajeeston,* and H. Fjellvåg

Center for Materials Sciences and Nanotechnology, Department of Chemistry, University of Oslo, P.O. Box 1033 Blindern, N-0315 Oslo, Norway

E-mail: ponniahv@kjemi.uio.no

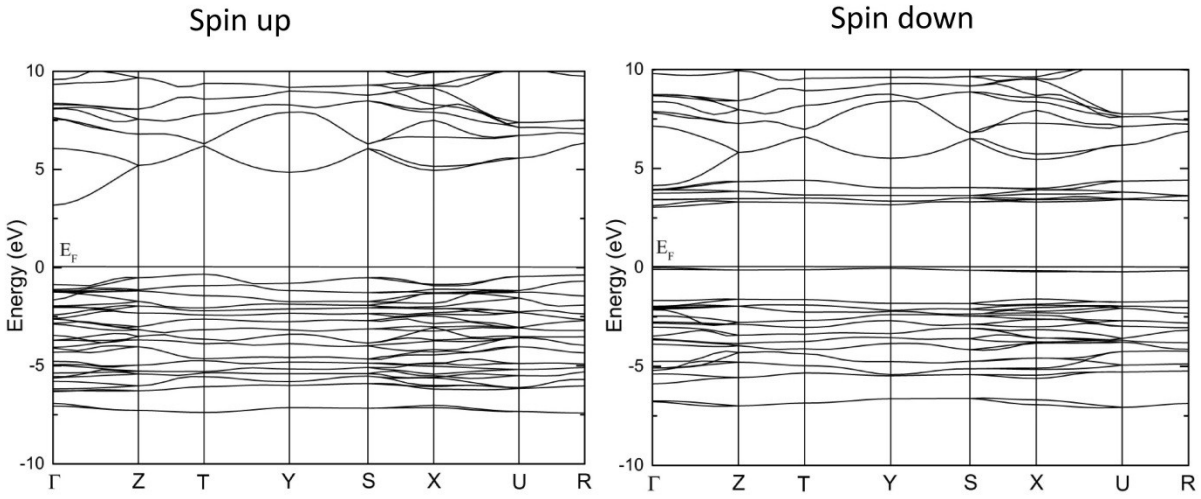

Fig.S1 Calculated electronic up-spin and down-spin band structure of Li_2FeSiO_4 in $Pmn2_1$ structure. The Fermi level is set to zero.

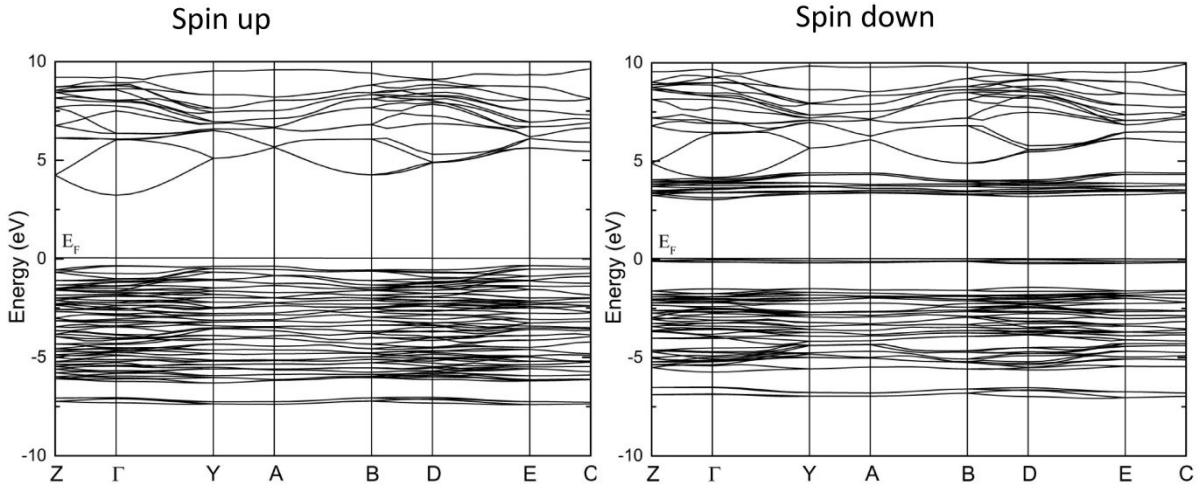

Fig.S2 Calculated electronic up-spin and down-spin band structure of Li_2FeSiO_4 in $P2_1$ structure. The Fermi level is set to zero.

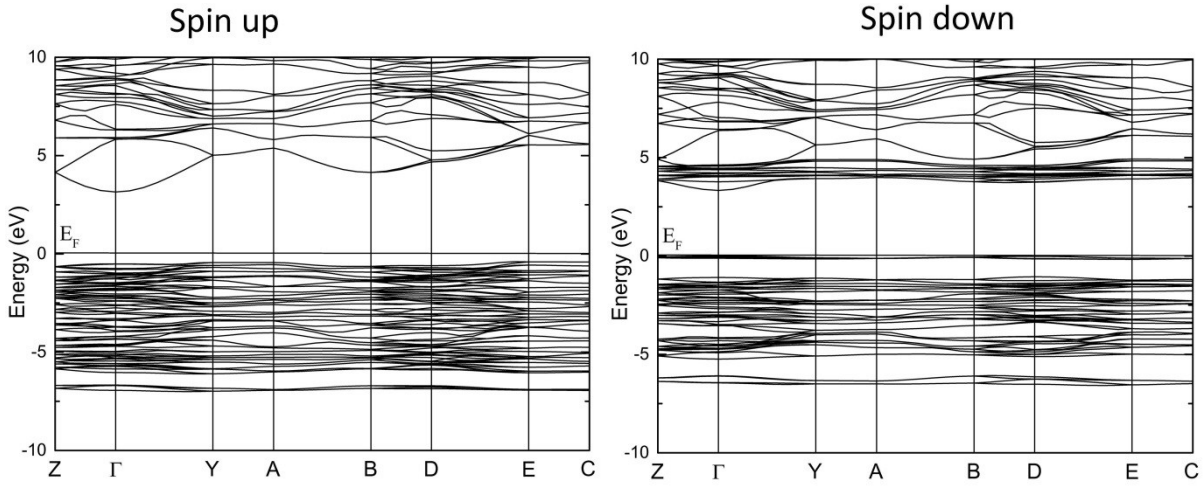

Fig.S3 Calculated electronic up-spin and down-spin band structure of Li_2FeSiO_4 in $P2_1/c$ structure. The Fermi level is set to zero.

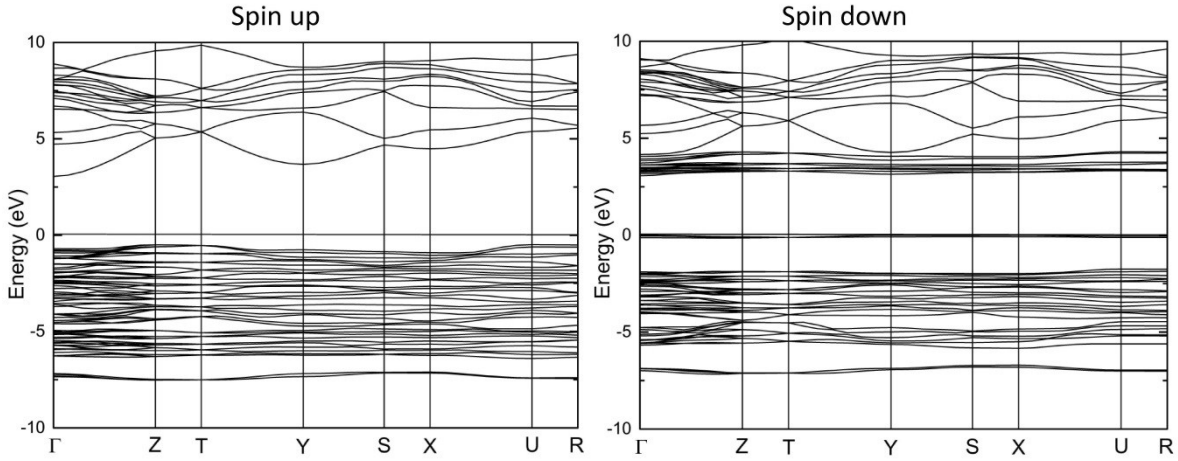

Fig.S4 Calculated electronic up-spin and down-spin band structure of Li_2FeSiO_4 in $Pbn2_1$ structure. The Fermi level is set to zero.

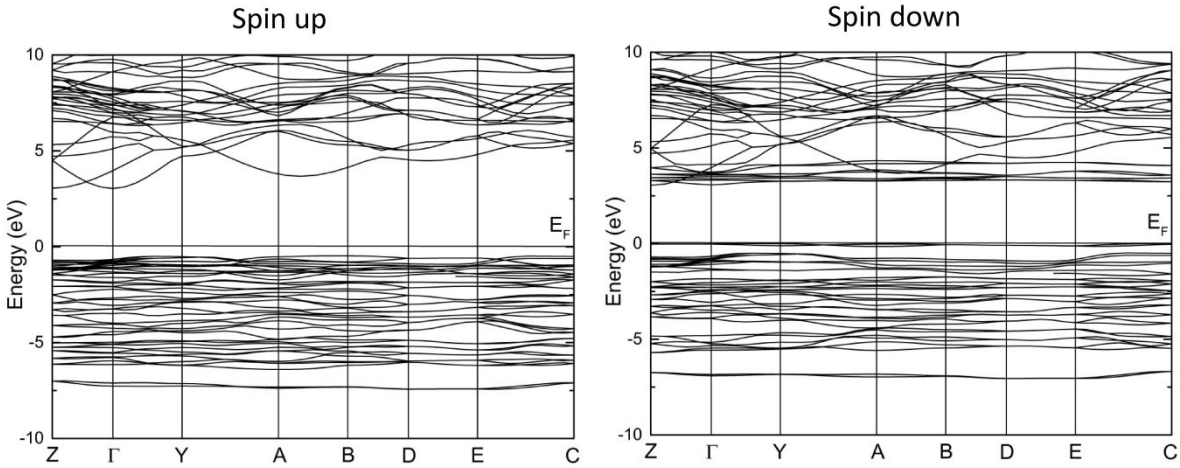

Fig.S5 Calculated electronic up-spin and down-spin band structure of Li_2FeSiO_4 in $Pmn2_1$-*mod* structure. According to the structural analysis the modified $Pmn2_1$ structure ($Pmn2_1$-*mod)* can be described in monoclinic (space group *Pc*; space group number 7) structure. The Fermi level is set to zero.

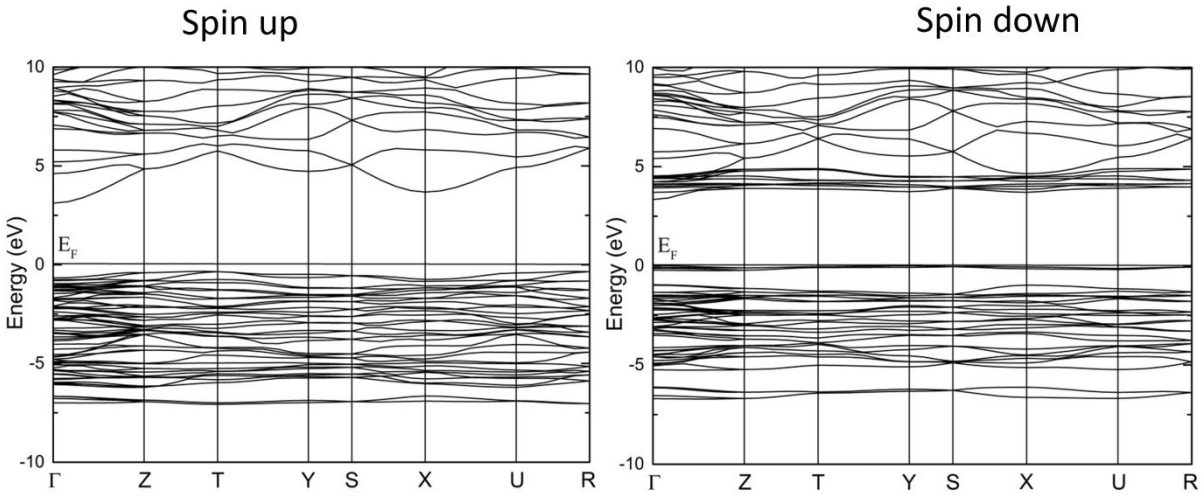

Fig.S6 Calculated electronic up-spin and down-spin band structure of Li_2FeSiO_4 in *Pmnb* structure. The Fermi level is set to zero.

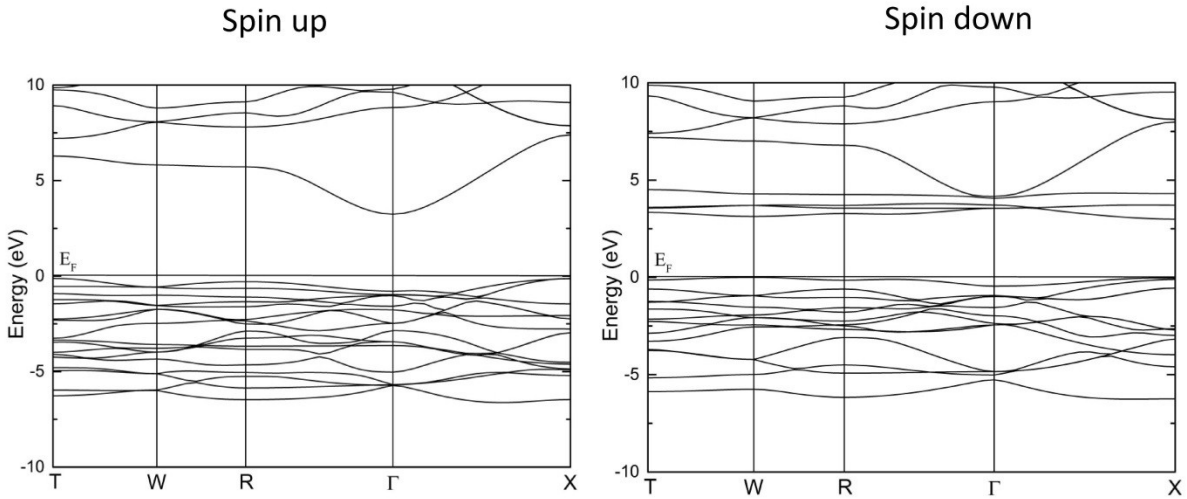

Fig. S7 Calculated electronic up-spin and down-spin band structure of Li_2FeSiO_4 in *I222* structure. The Fermi level is set to zero.

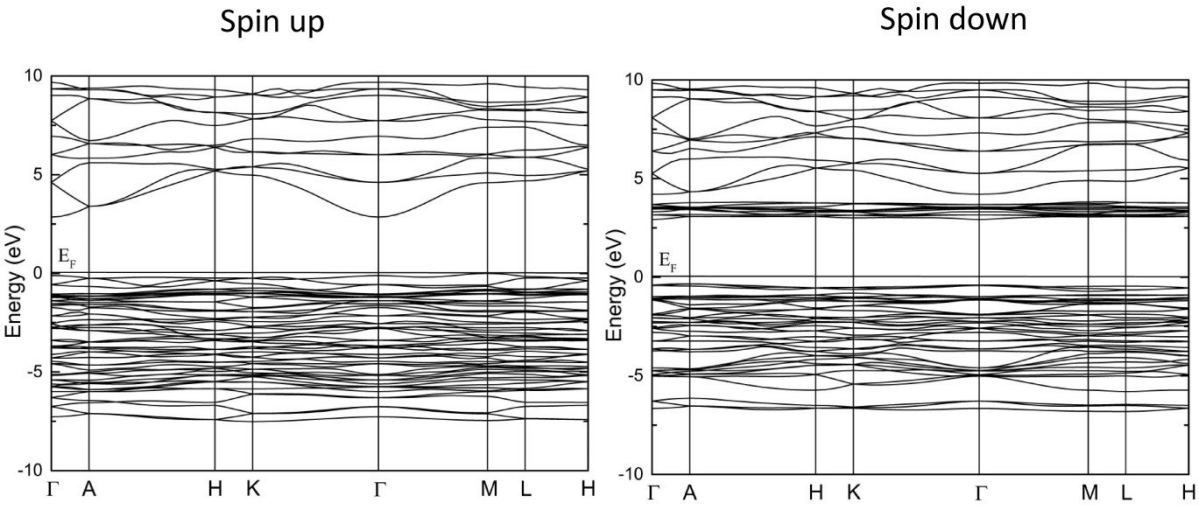

Fig.S8 Calculated electronic up-spin and down-spin band structure of Li_2FeSiO_4 in P3121 structure. The Fermi level is set to zero.

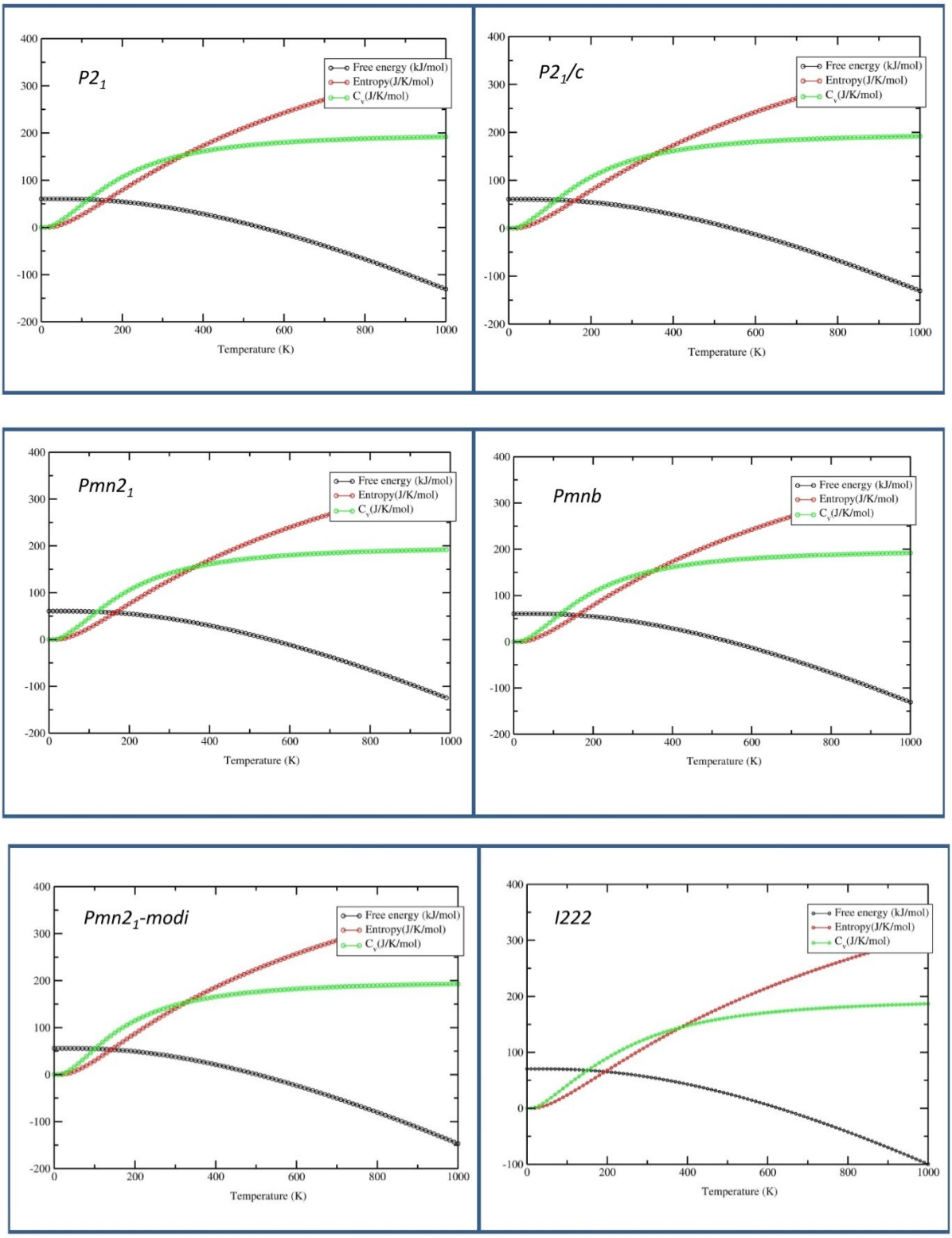

Fig.S9 Calculated free energy (in kJ/mol), entropy (in J/K/mol.) and lattice heat capacity (Cv; in J/K/mol.) as a function of temeperature for Li_2FeSiO_4 in *$P2_1$, $P2_1/c$, $Pmn2_1$, Pmnb, $Pmn2_1$-modi* and *I222* modifications.