Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Understanding the electrochemical properties of A_2MSiO_4 (A = Li, Na; M = Fe, Mn, Co and Ni) and Na doping effect on Li_2MSiO_4 from first-principle calculations

Yuhan Li,[ab] Weiwei Sun,[d] Jing Liang,[ac] Hao Sun,[ac] Igor Di Marco,[d] Lei Ni[b], Shuwei Tang*[ac] and Jingping Zhang*[a]

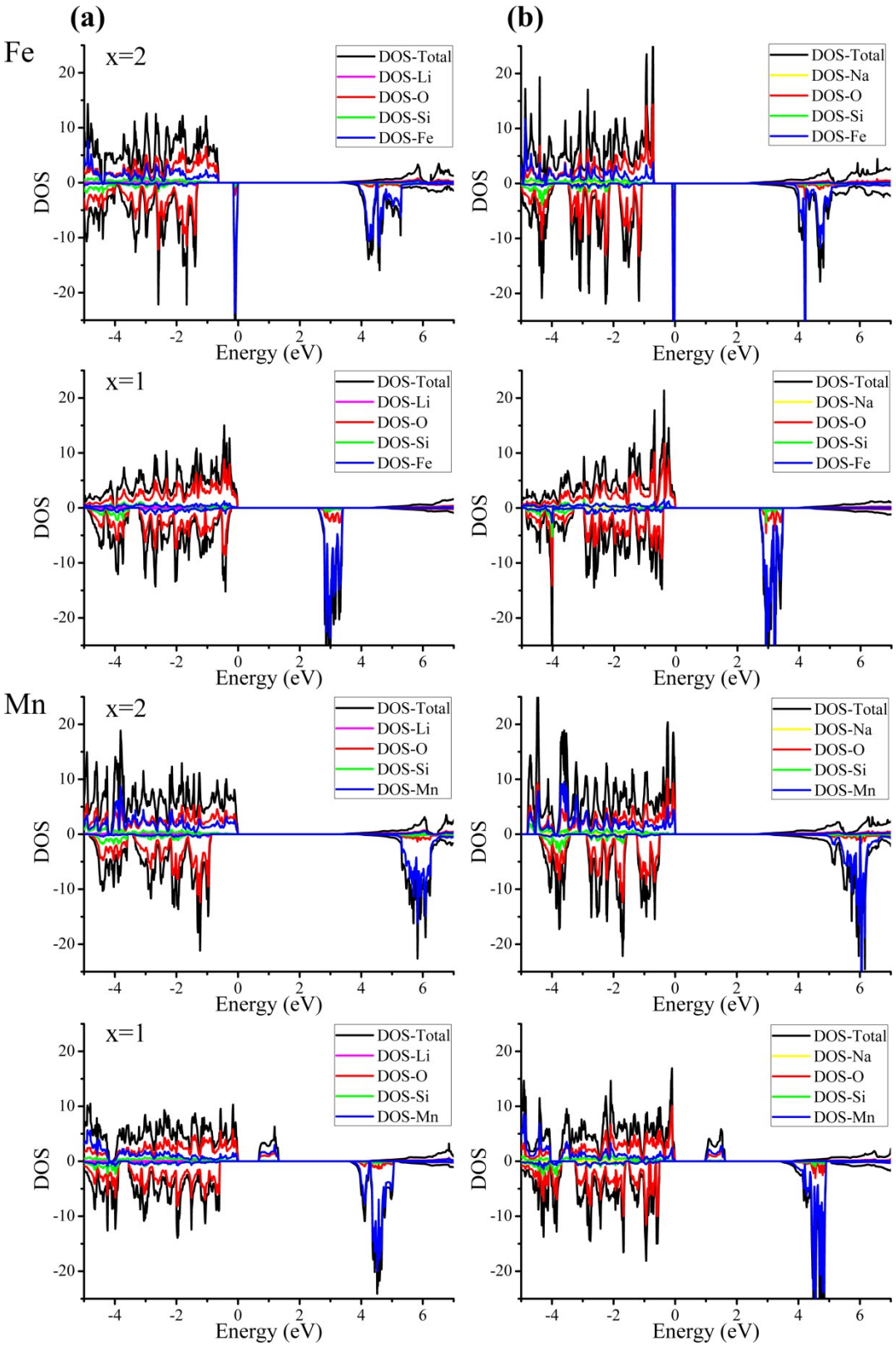
[a] *Institute of Functional Material, Faculty of Chemistry, Northeast Normal University, Changchun, Jilin 130024, China.*

**E-mail: tangsw911@nenu.edu.cn, jpzhang@nenu.edu.cn*

[b] *College of Chemistry and Biology, Beihua University, Jilin, Jilin 132013, China.*

[c] *National & Local United Engineering Lab for Power Battery, Northeast Normal University, Changchun, Jilin 130024, China.*

[d] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120 Uppsala, Sweden.*


(a)
(b)
Fe
x=2
x=1
Mn
x=2
x=1
DOS-Total
DOS-Li
DOS-Na
DOS-O
DOS-Si
DOS-Fe
DOS-Mn
DOS
Energy (eV)

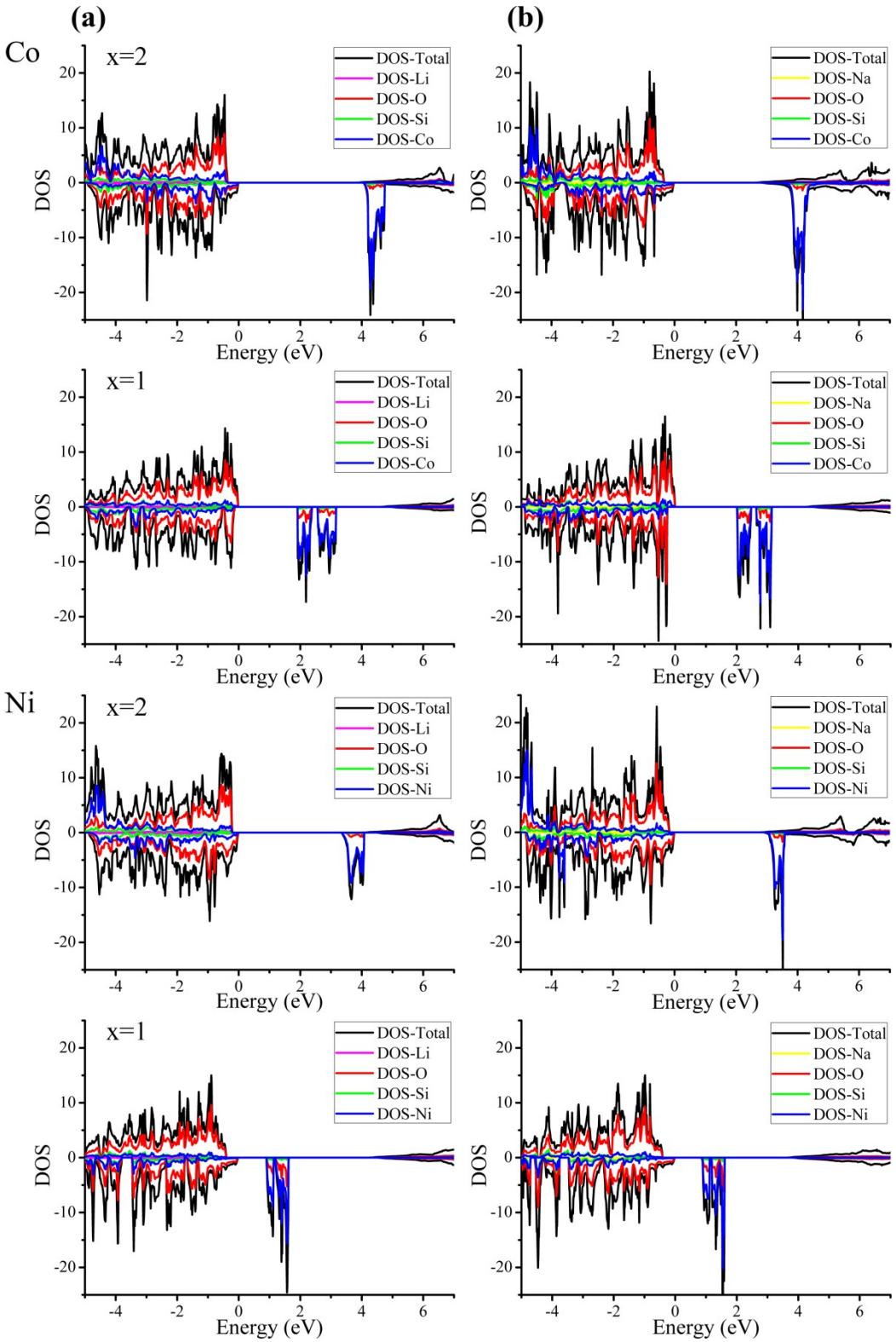


Fig. S1 Calculated local density of states for (a) Li_xMSiO_4 and (b) Na_xMSiO_4 (x = 1 and 2 and M = Fe, Mn, Co and Ni). The total density of states is figured in a black, Li is in pink, Na is in yellow, O is in red line, Si is in green and M is in blue line

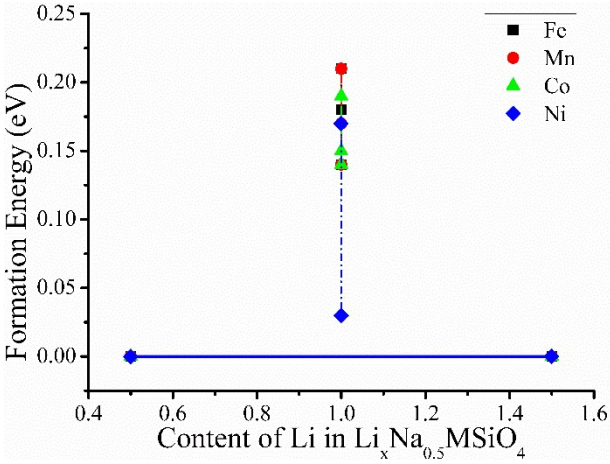


Fig. S2 Calculated formation energies for possible intermediate phases of $Li_1Na_{0.5}MSiO_4$ (M = Fe, Mn, Co and Ni)

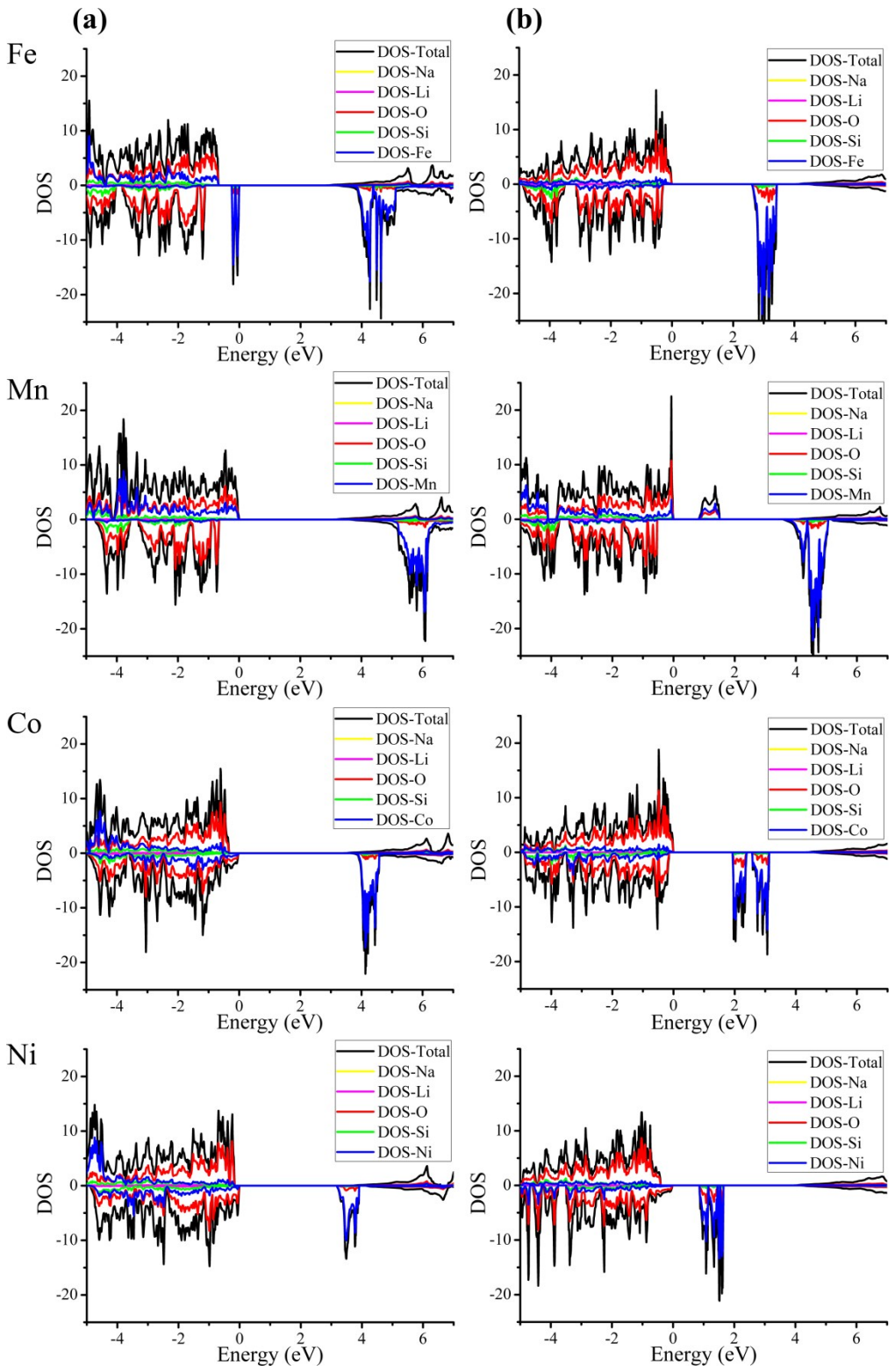


Fig. S3 Calculated local density of states for (a) $Li_{1.5}Na_{0.5}MSiO_4$ and (b) $Li_{0.5}Na_{0.5}MSiO_4$ (M = Fe, Mn, Co and Ni)

by a black line, Li with pink, O with red, P with green and V with blue.