

Electronic Supplementary Information

Tuning the electronic and magnetic properties of lizardite clay by chemical substitution

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1 Formation Energy

Table 1: Formation Energy for $A_3(\text{Si}_2\text{O}_5)\text{X}_4$, where X=OH, F, Cl, using Eq.(1)

| A | Formation Energy (eV) | | |
|----|---|--|---|
| | $A_3(\text{Si}_2\text{O}_5)\text{OH}_4$ | $A_3(\text{Si}_2\text{O}_5)\text{F}_4$ | $A_3(\text{Si}_2\text{O}_5)\text{Cl}_4$ |
| Mg | -63.79 | -70.80 | -53.11 |
| Ca | -65.35 | | |
| Mn | -61.30 | -67.67 | -49.96 |
| Fe | -62.17 | -68.04 | -51.43 |
| Ni | -59.57 | -65.00 | -51.34 |
| Zn | -54.21 | | |

2 Crystal Structure of the New Compounds after calculations with density functional theory (DFT)

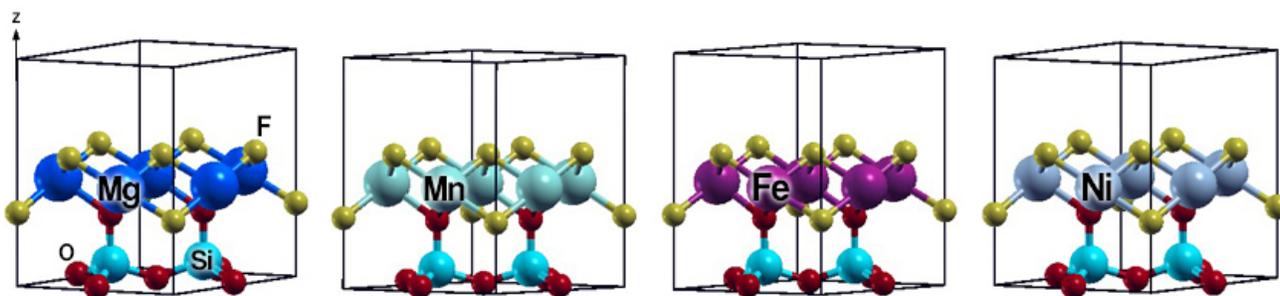


Figure 1: Crystal structure of $A_3(\text{Si}_2\text{O}_5)\text{F}_4$, where A = Mg, Mn, Fe and Ni.

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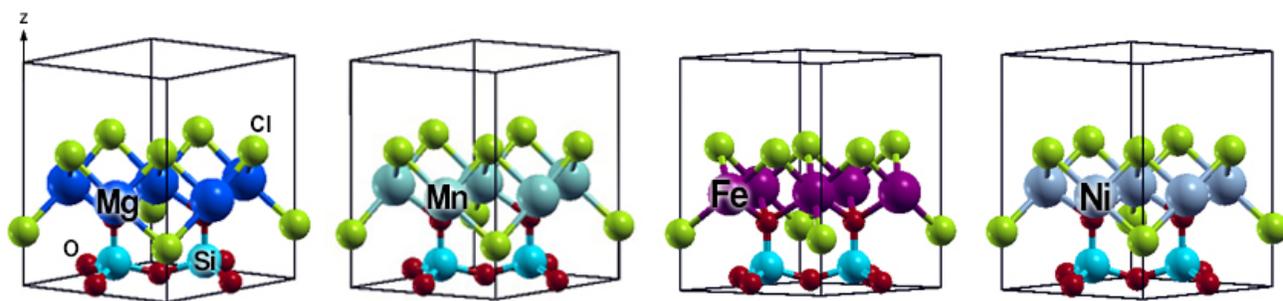


Figure 2: Crystal structure of $A_3(Si_2O_5)Cl_4$, where $A = Mg, Mn, Fe$ and Ni .