# Supplementary Information

TABLE I: Theoretical specific capacity (in mAh/g-$CaMO_3$) of some of the investigated $CaMO_3$ perovskites assuming 100% calcium de-intercalation

| TM | Mo | Cr | Mn | Fe | Co | Ni |
|---|---|---|---|---|---|---|
| Theoretical specific capacities (mAh/g) | 291 | 383 | 375 | 372 | 364 | 365 |

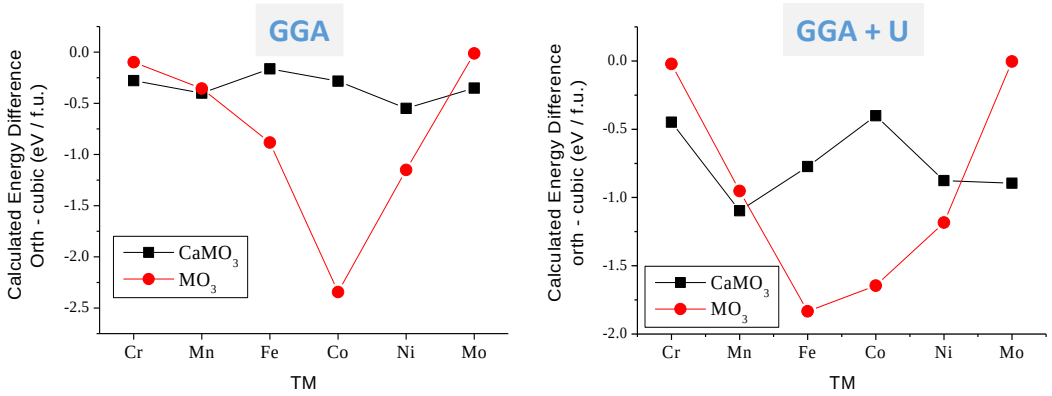


**Figure 1.**- Calculated energy difference between the cubic and the orthorhombic symmetry for $CaMO_3$ (black squares) and $MO_3$ (red circles) perovskites within the GGA approximation (left) and the GGA+U (right).

**TABLE II.** Calculated lattice parameters (in Å) for orthorhombic $MO_3$ structures (S.G. *Pnma*) within the GGA and the GGA+U method.

| TM | Approximant | *a* | *b* | *c* |
|---|---|---|---|---|
| Mo | GGA | 5.383 | 7.539 | 5.283 |
| | GGA+U | 5.388 | 7.547 | 5.289 |
| Cr | GGA | 4.940 | 6.938 | 4.823 |
| | GGA+U | 4.493 | 6.943 | 4.825 |
| Mn | GGA | 4.839 | 6.802 | 4.695 |
| | GGA+U | 4.831 | 6.909 | 4.766 |
| Fe | GGA | 5.356 | 6.015 | 4.720 |
| | GGA+U | 5.625 | 6.211 | 5.165 |
| Co | GGA | 4.578 | 6.878 | 4.604 |
| | GGA+U | 4.834 | 6.957 | 4.881 |
| Ni | GGA | 4.753 | 6.732 | 4.704 |
| | GGA+U | 4.728 | 6.741 | 4.673 |

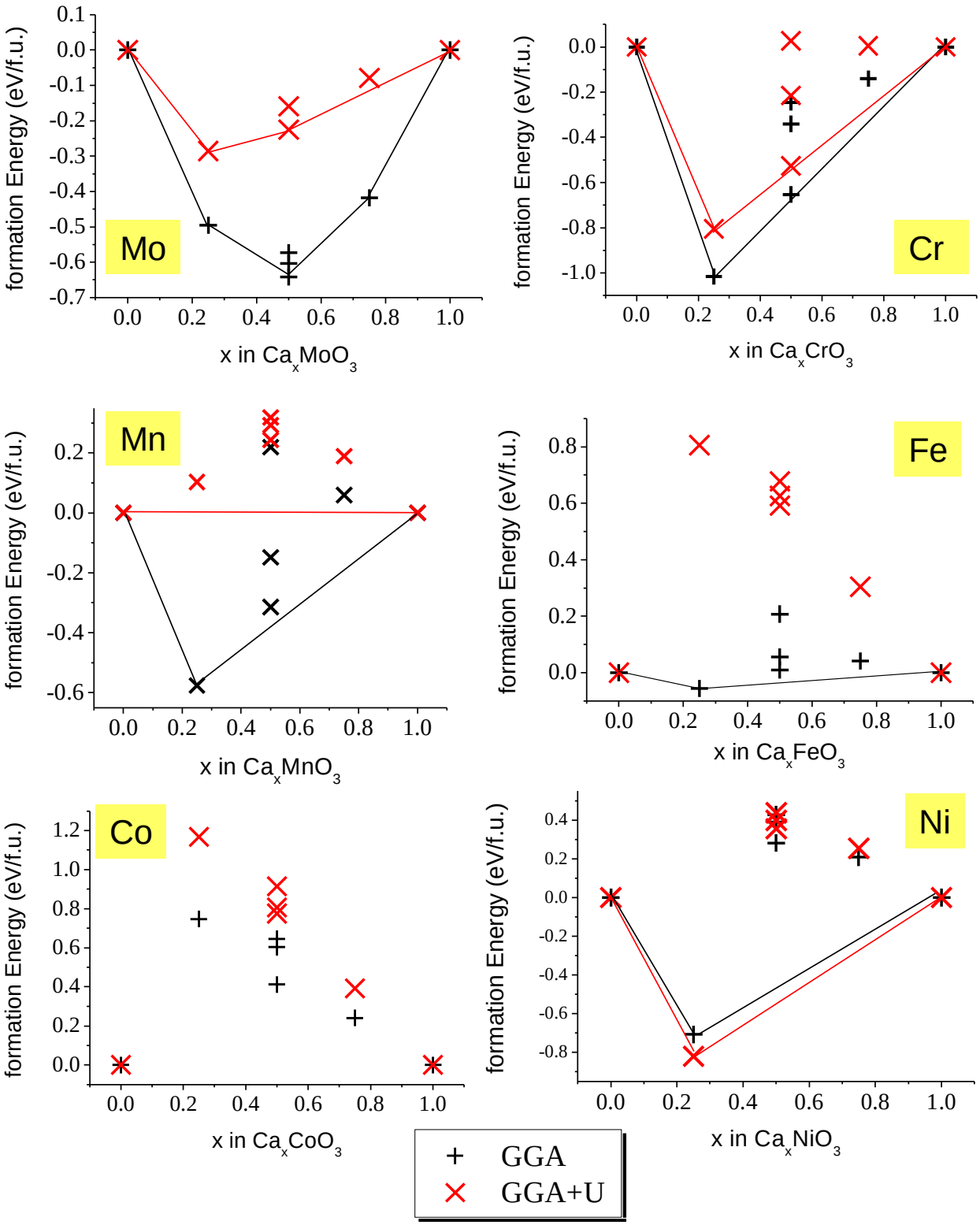


**Figure 2.**- Calculated formation energies of ordered $Ca_xMO_3$ structures as a function of the calcium concentration. Red for GGA+U and black for GGA.