Supporting Information

High throughput Screening of TMOCl Cathode Materials based on Full-Cell System for Chloride-Ion Batteries

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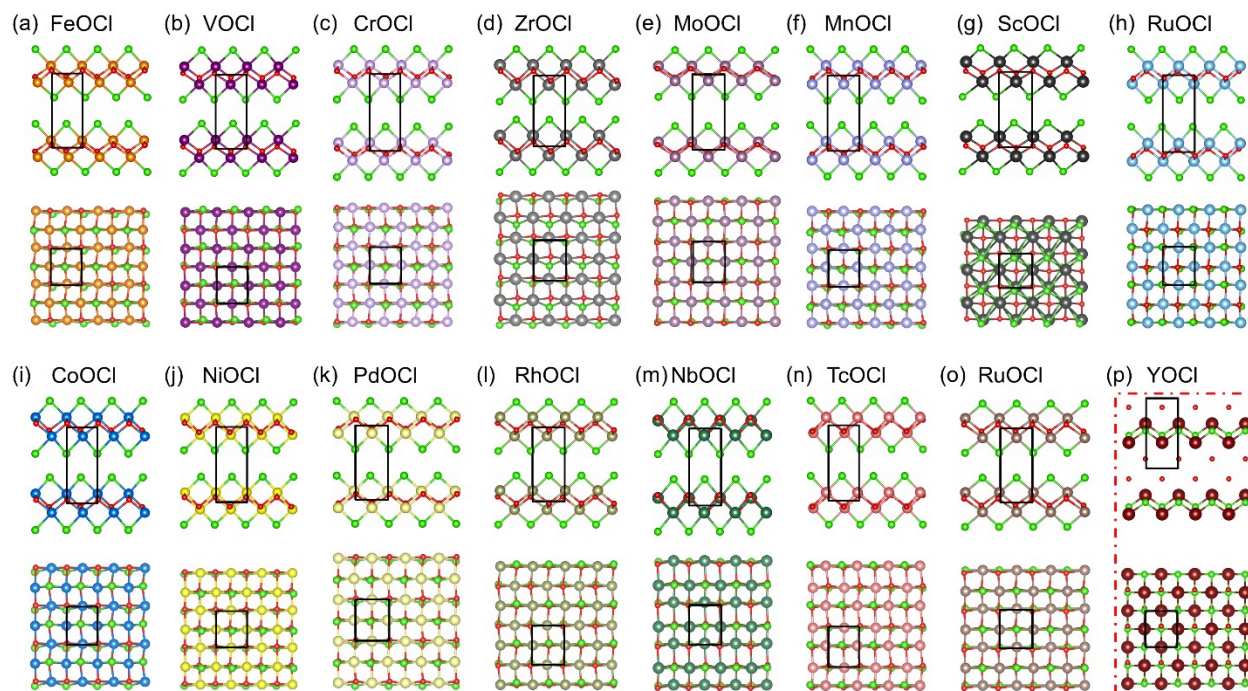
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Figure S1. The simulated structure of (a) FeOCl, (b) VOCl, (c) CrOCl, (d) ZrOCl, (e) MoOCl, (f) MnOCl, (g) ScOCl, (h) RuOCl, (i) CoOCl, (j) NiOCl, (k) PdOCl, (l) RhOCl, (m) NbOCl, (n) TcOCl, (o) RuOCl, and (p) YOCl at 600 K after 10 ps.
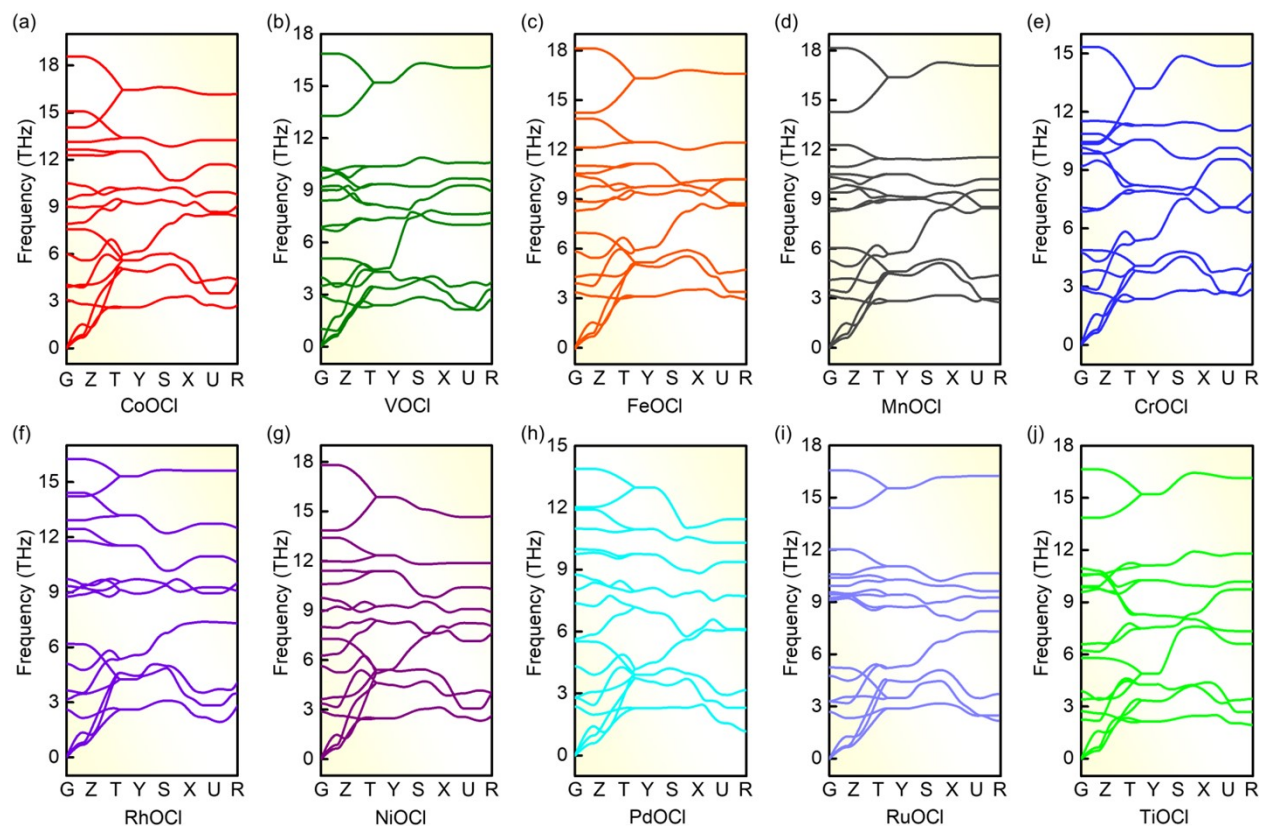
Figure S2. Phonon band structure of (a) CoOCl, (b) VOCl, (c) FeOCl, (d) MnOCl, (e) CrOCl, (f) RhOCl, (g) NiOCl, (h) PdOCl, (i) RuOCl, and (j) TiOCl.
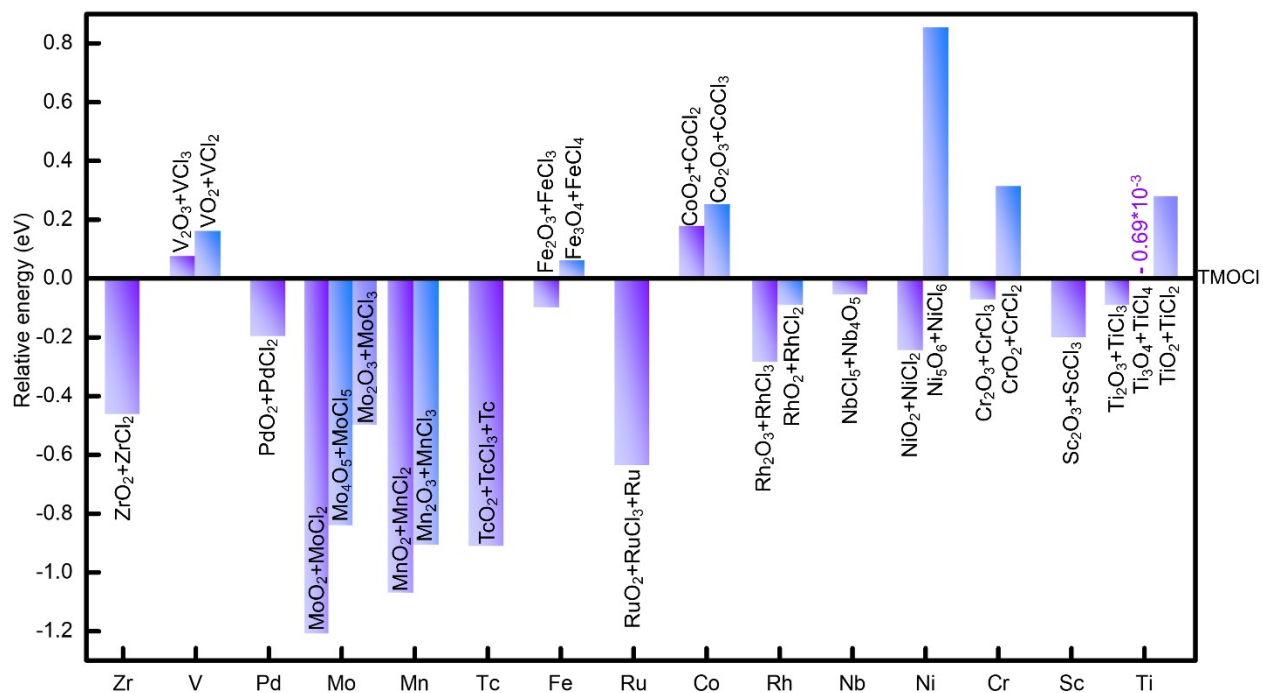
Figure S3. The relative energy between TMOCl and their possible decomposition products, where TMOCl is used as a reference.
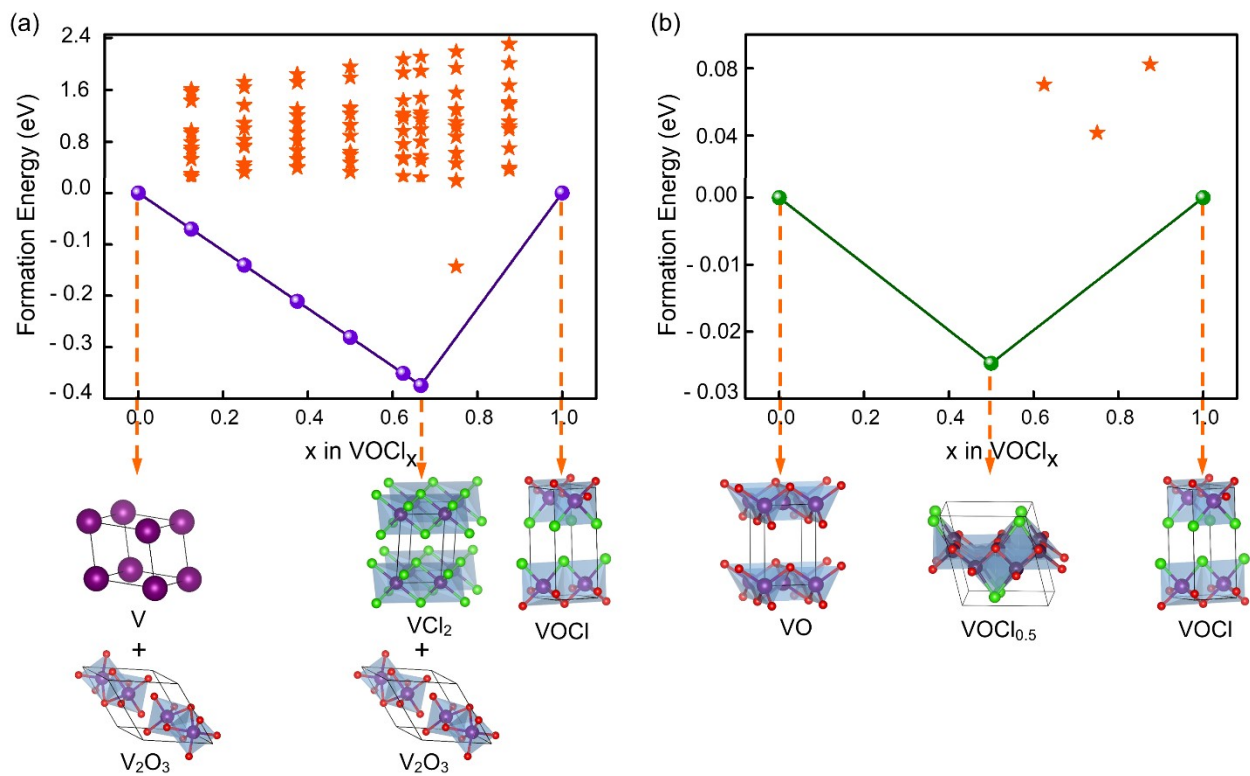
Figure S4. Formation energy of VOCl$_x$ following (a) decomposition reaction and (b) deintercalation reaction.
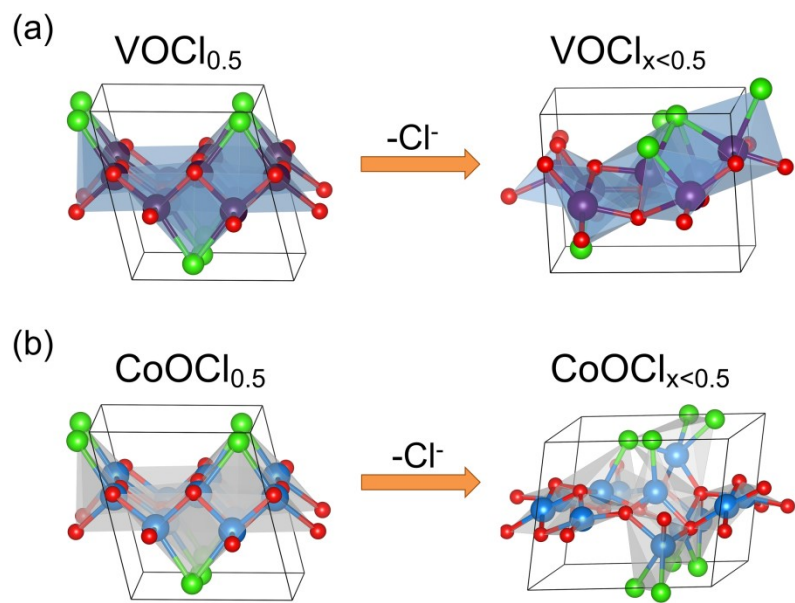
(a)

VOCl$_{0.5}$ VOCl$_{x<0.5}$

-Cl$^-$

(b)

CoOCl$_{0.5}$ CoOCl$_{x<0.5}$

-Cl$^-$

Figure S5. Structures of (a) VOCl$_{0.5}$ and VOCl$_{0.375}$, (b) CoOCl$_{0.5}$ and CoOCl$_{0.375}$.
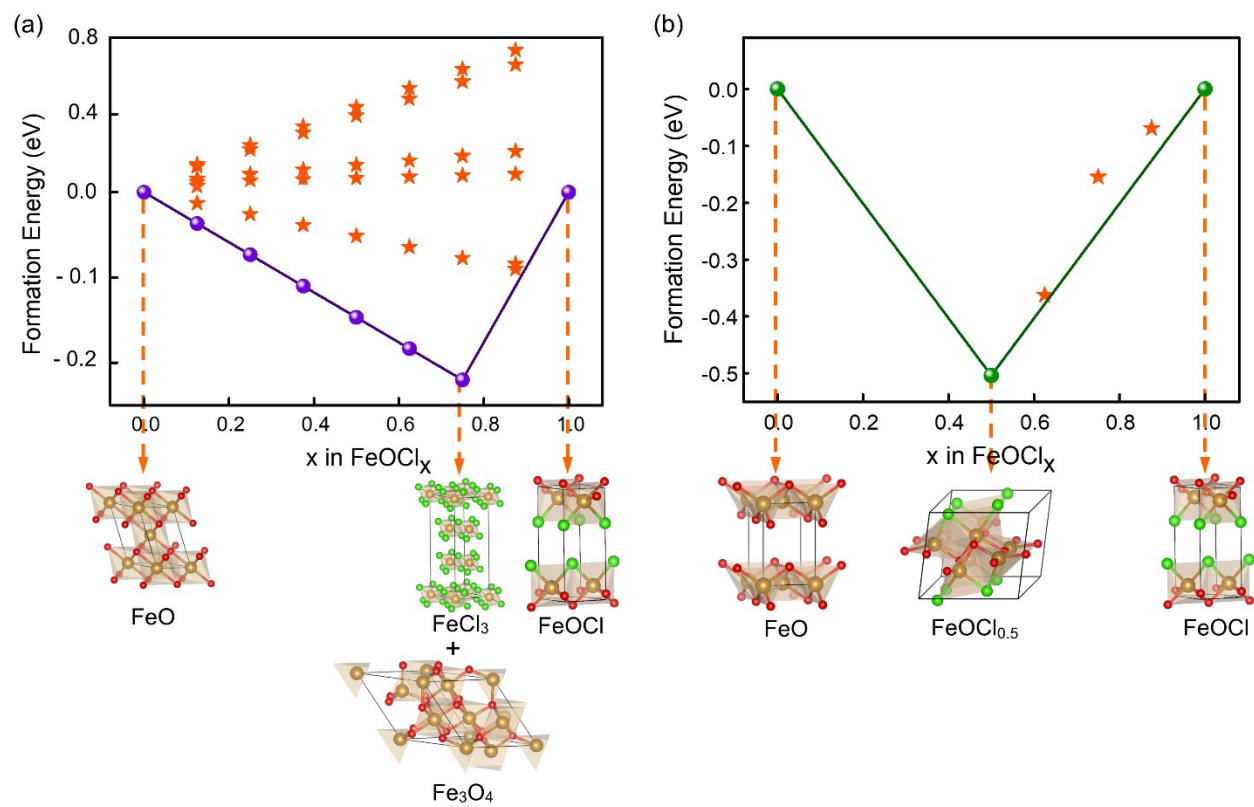
Figure S6. Formation energy of FeOClₓ following (a) decomposition reaction and (b) deintercalation reaction.
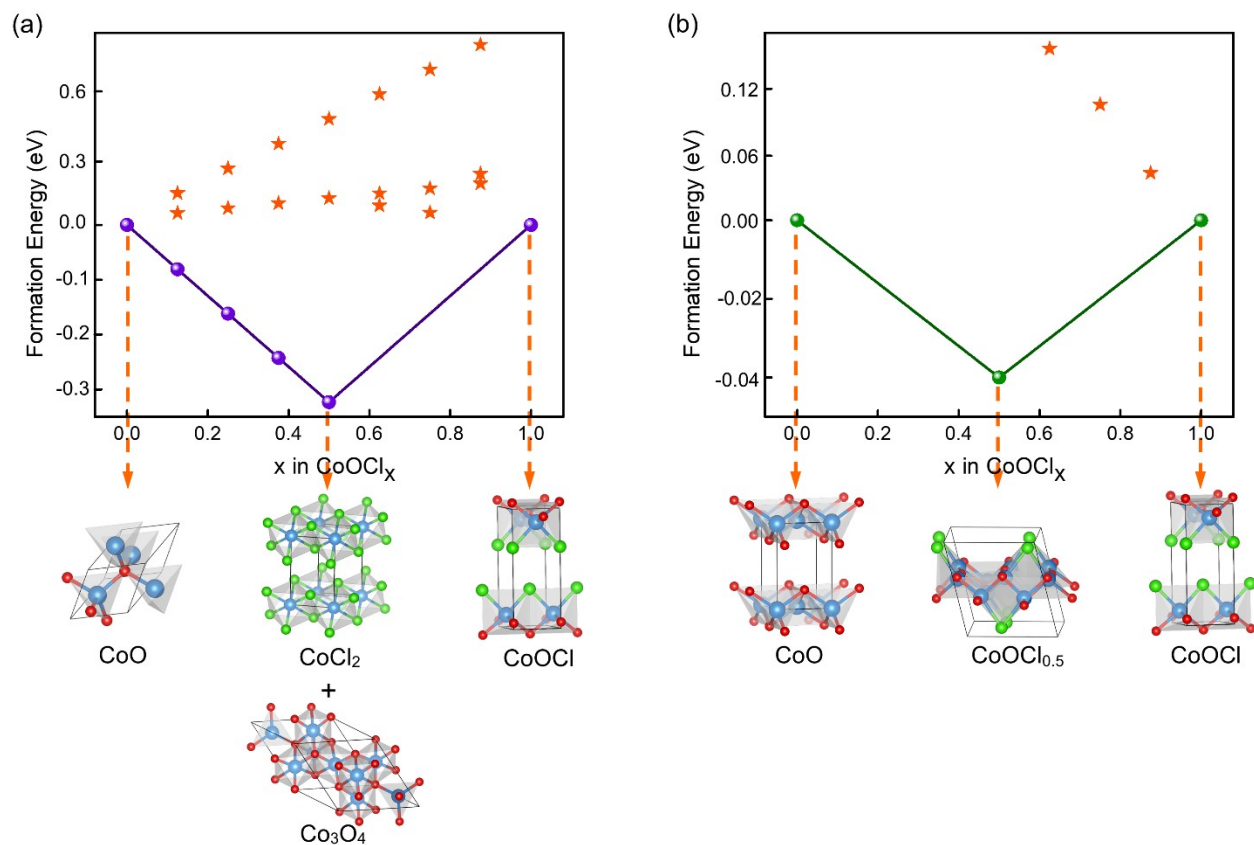
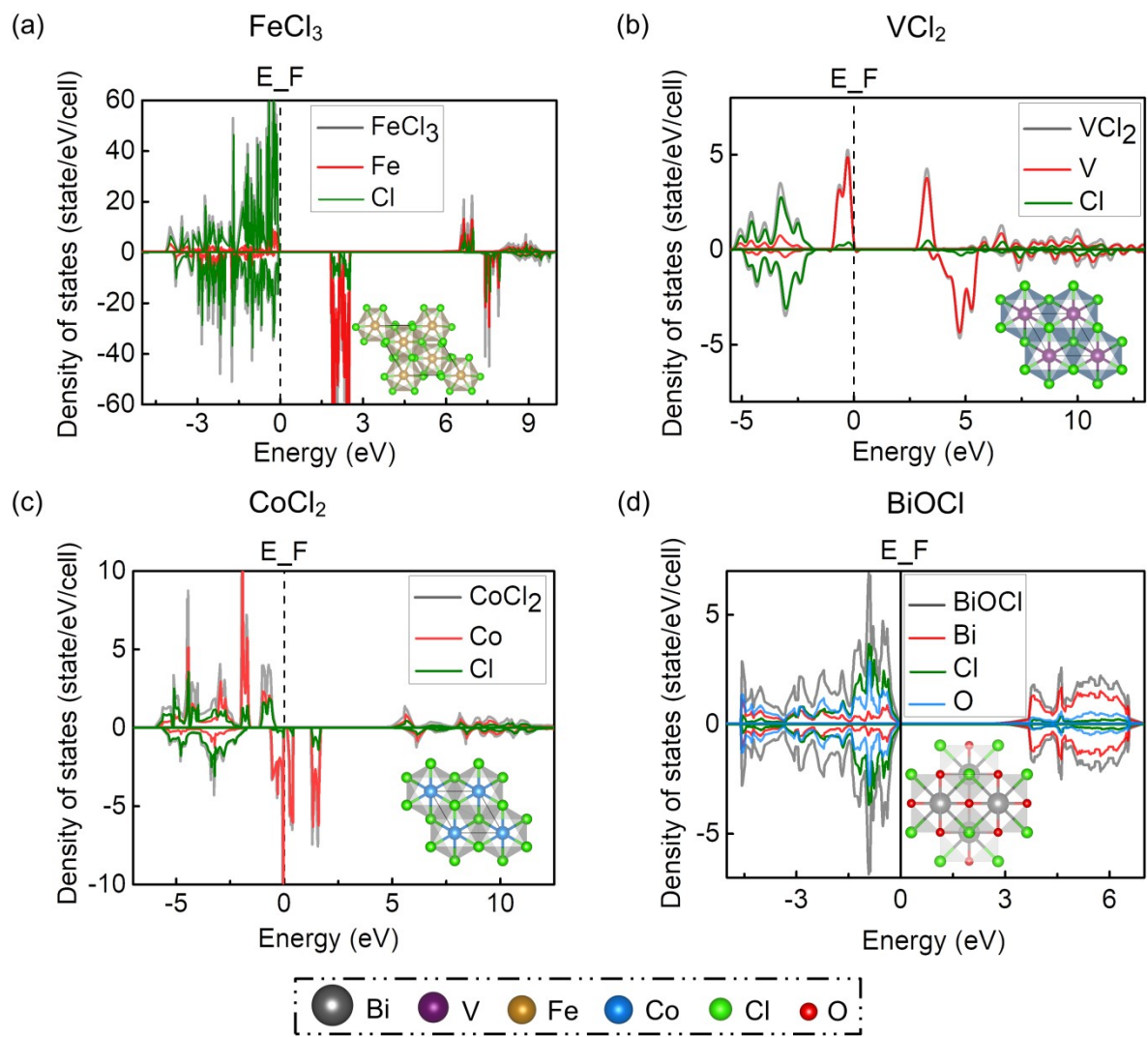**Figure S7.** Formation energy of CoOCl$_x$ following (a) decomposition reaction and (b) deintercalation reaction.

Figure S8. Density of states of (a) FeCl$_3$, (b) VCl$_2$, (c) CoCl$_2$, and (d) BiOCl.