

Supplementary Information

High-throughput Discovery of Magnetic Rare-earth–Transition-metal Alloys

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1 Binary convex hull diagrams

Figures S1–S6 show the DFT convex hull diagrams for each binary R-TM chemical system. Candidate structures with $E_{\text{hull}}^{\text{DFT-ref}} < 0.1$ eV/atom are plotted alongside Materials Project reference phases.

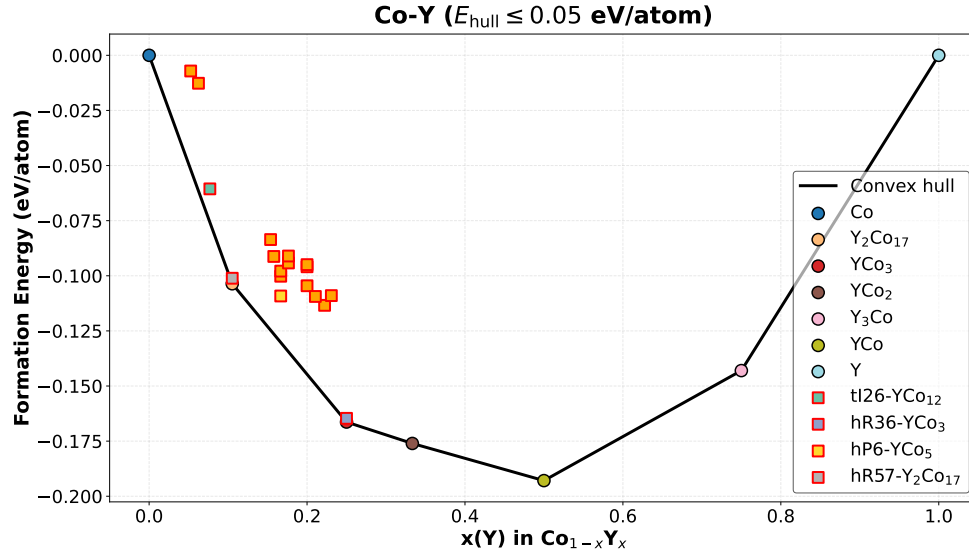


Figure S1: Convex hull for the Co–Y binary system.

2 Ternary convex hull diagrams

Figures S7–S36 show ternary convex hull cross-sections for each R-T-T' system.

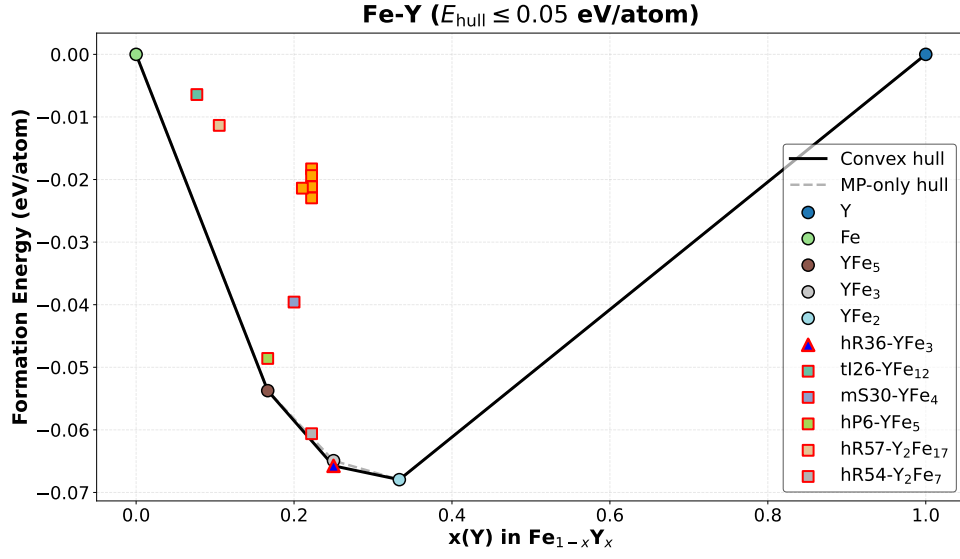


Figure S2: Convex hull for the Fe–Y binary system.

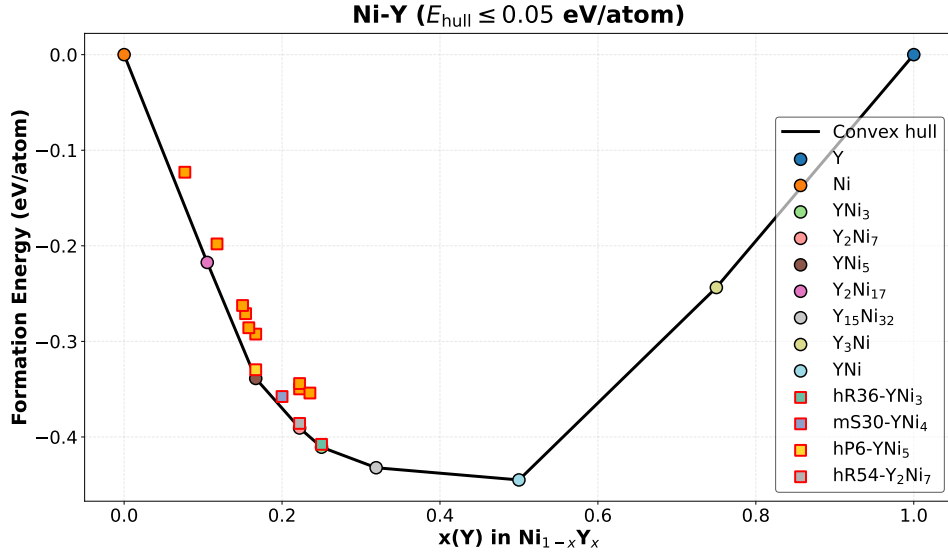


Figure S3: Convex hull for the Ni–Y binary system.

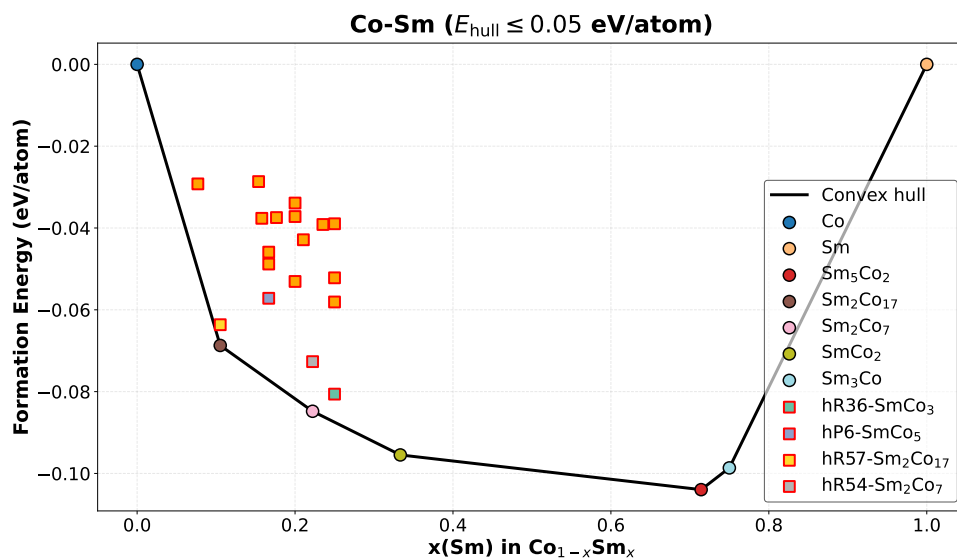


Figure S4: Convex hull for the Co–Sm binary system.

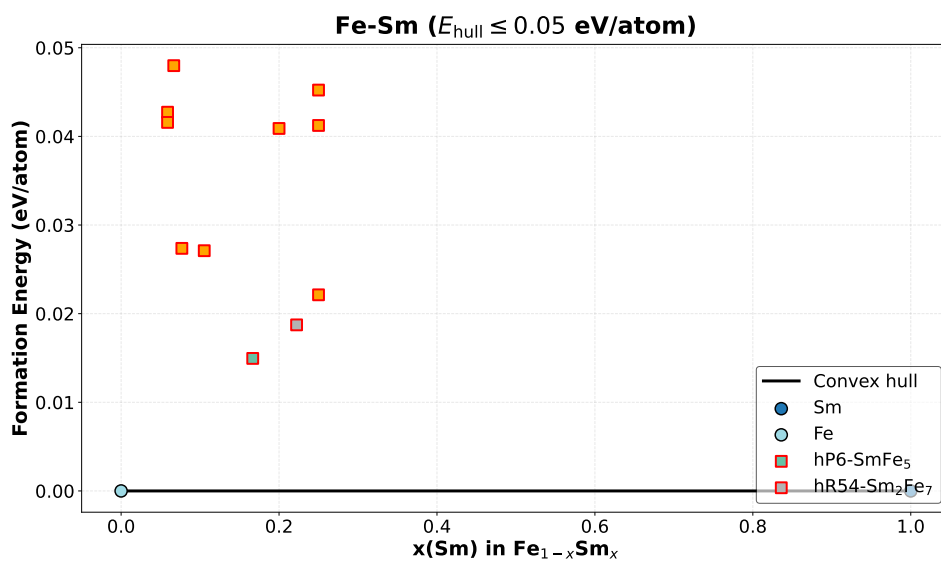


Figure S5: Convex hull for the Fe–Sm binary system.

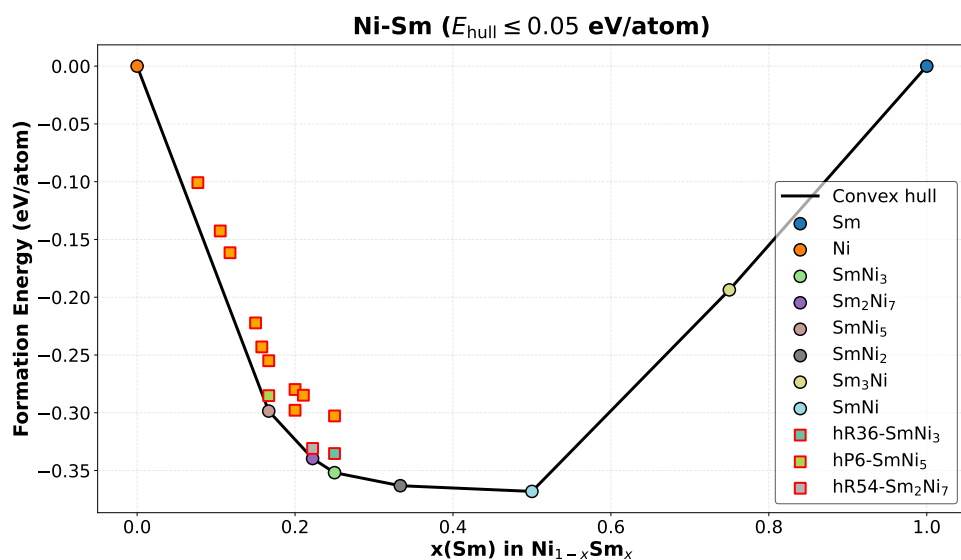


Figure S6: Convex hull for the Ni-Sm binary system.

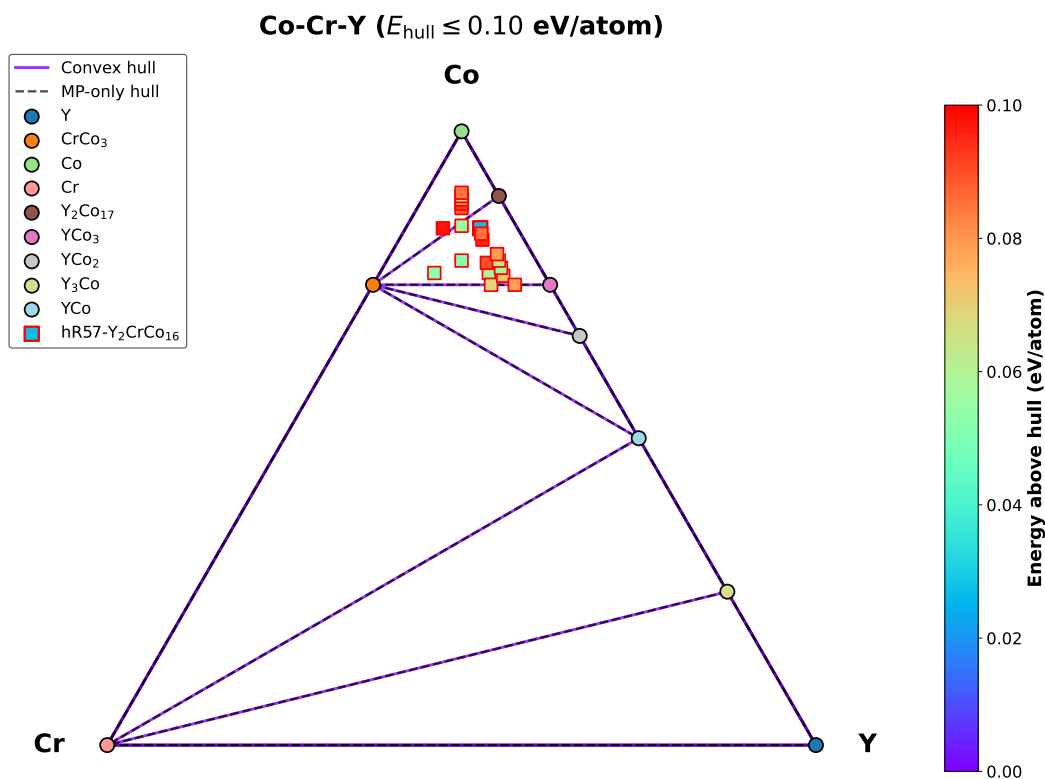


Figure S7: Ternary hull for the Co-Cr-Y system.

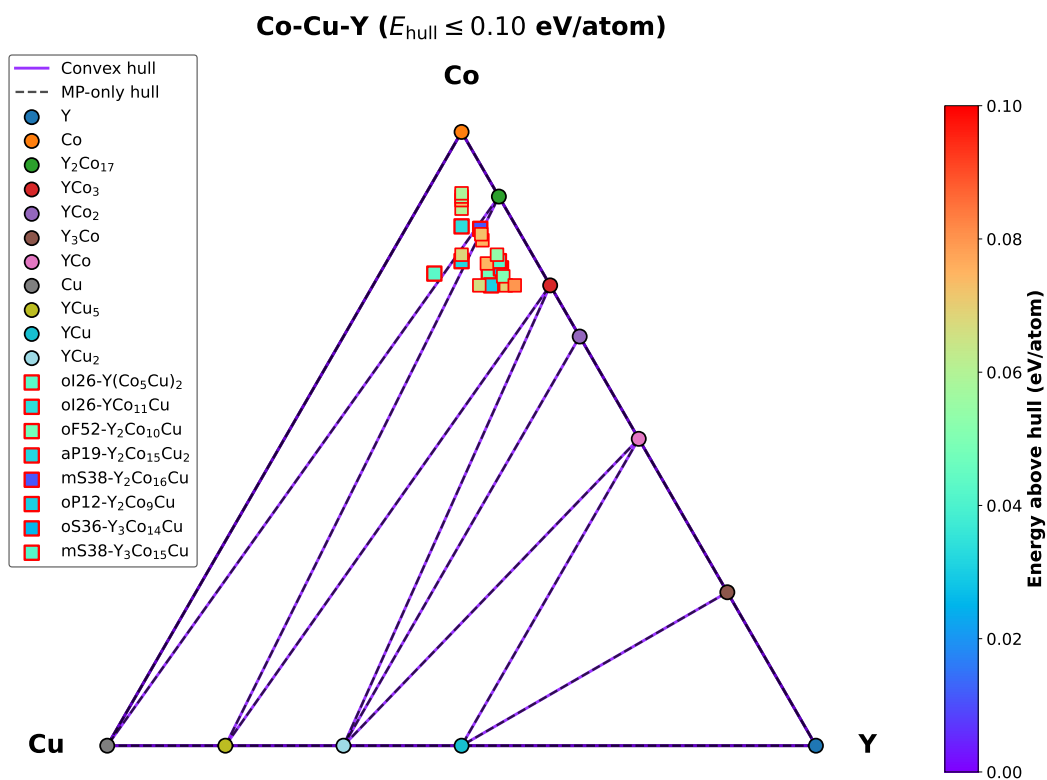


Figure S8: Ternary hull for the Co–Cu–Y system.

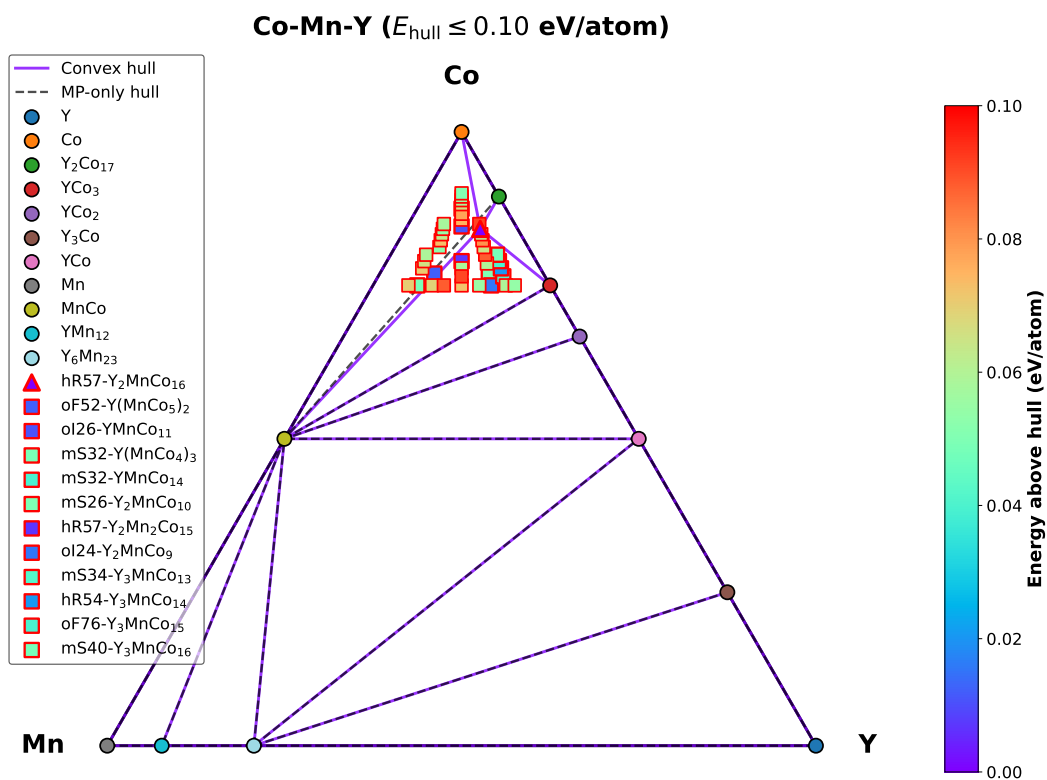


Figure S9: Ternary hull for the Co–Mn–Y system.

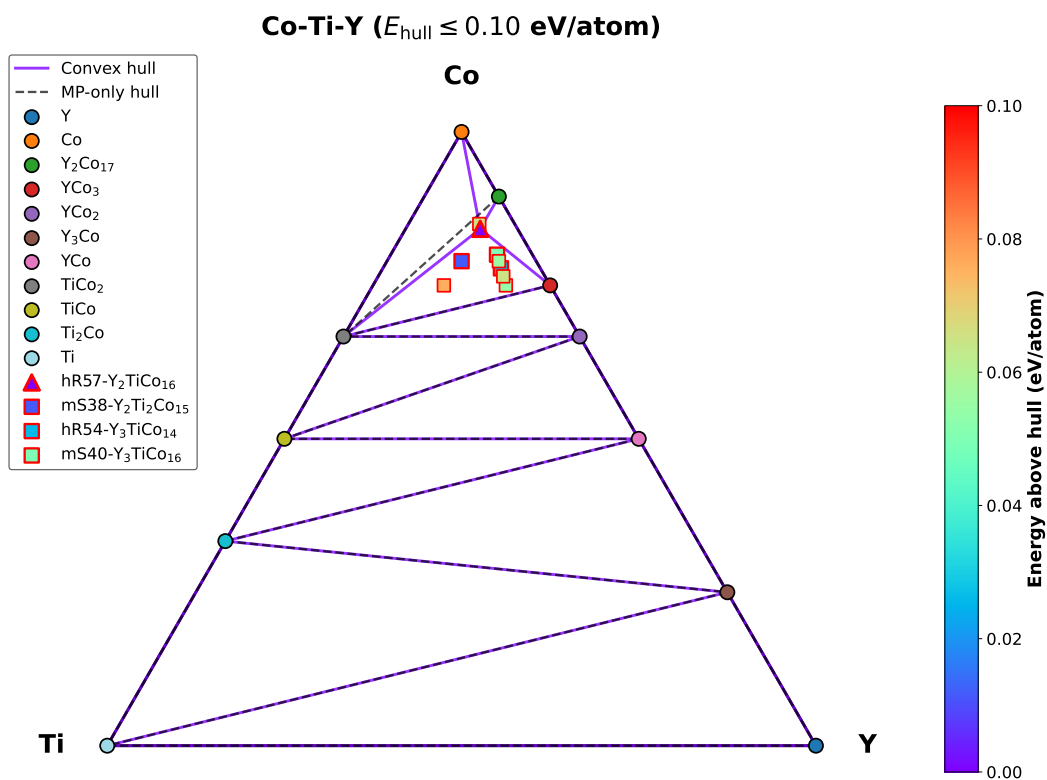


Figure S10: Ternary hull for the Co-Ti-Y system.

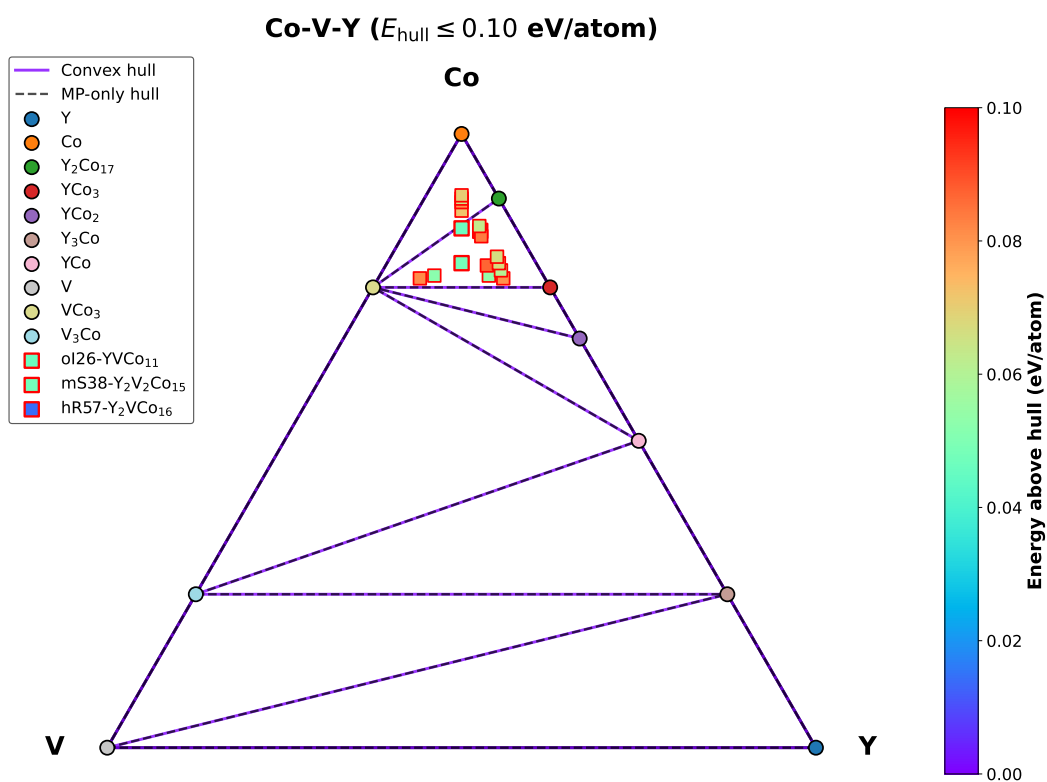


Figure S11: Ternary hull for the Co-V-Y system.

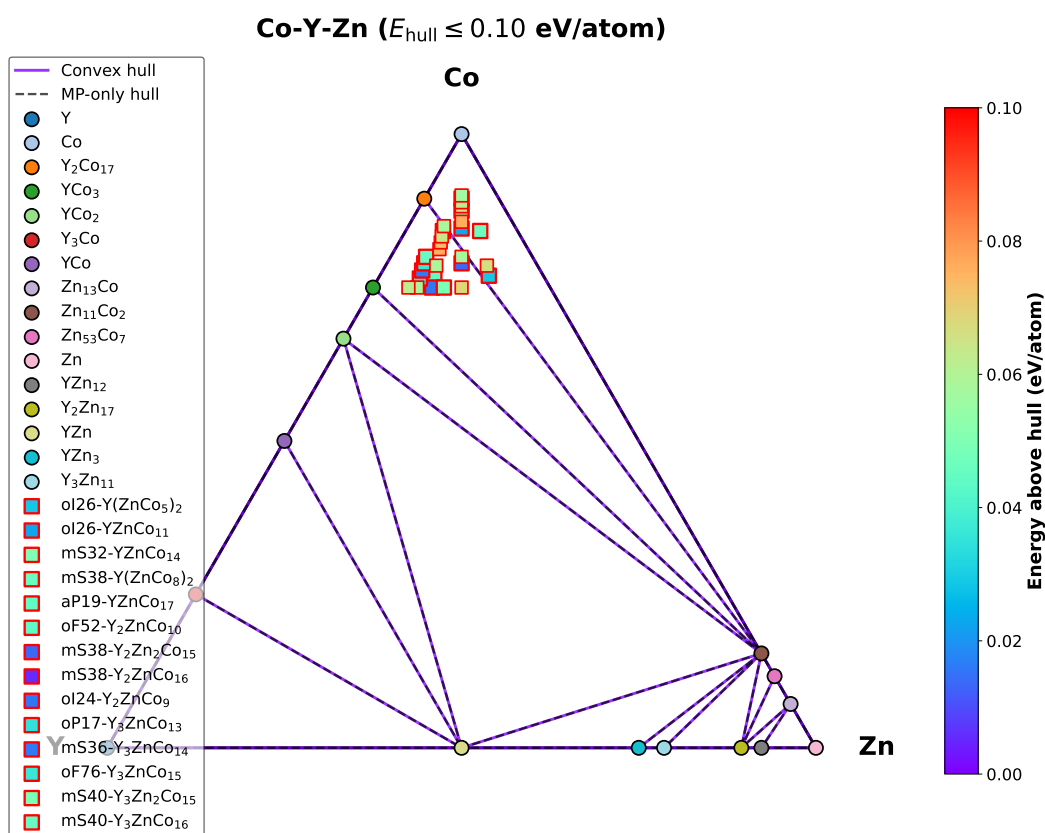


Figure S12: Ternary hull for the Co-Y-Zn system.

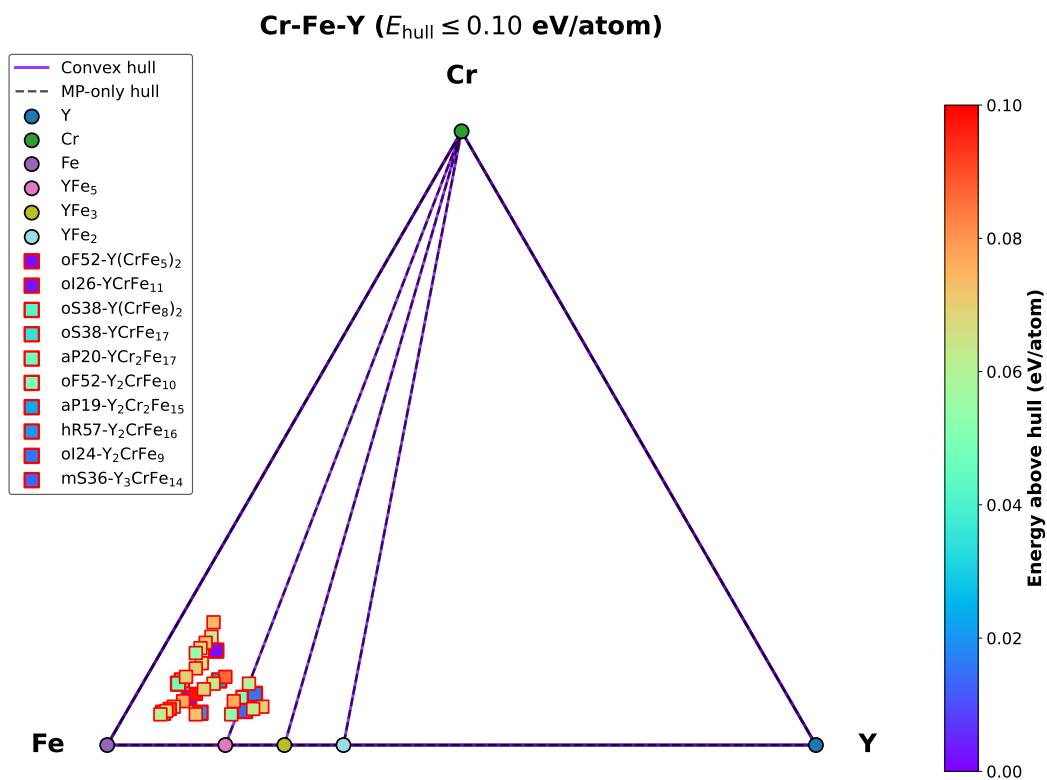


Figure S13: Ternary hull for the Cr–Fe–Y system.

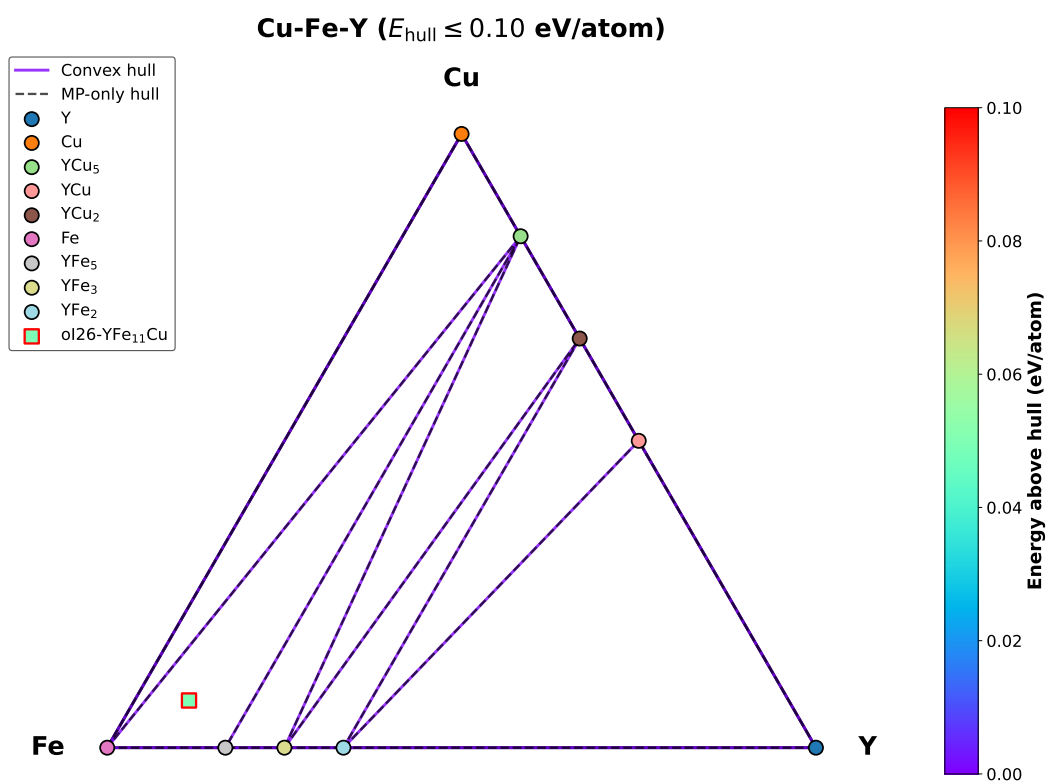


Figure S14: Ternary hull for the Cu-Fe-Y system.

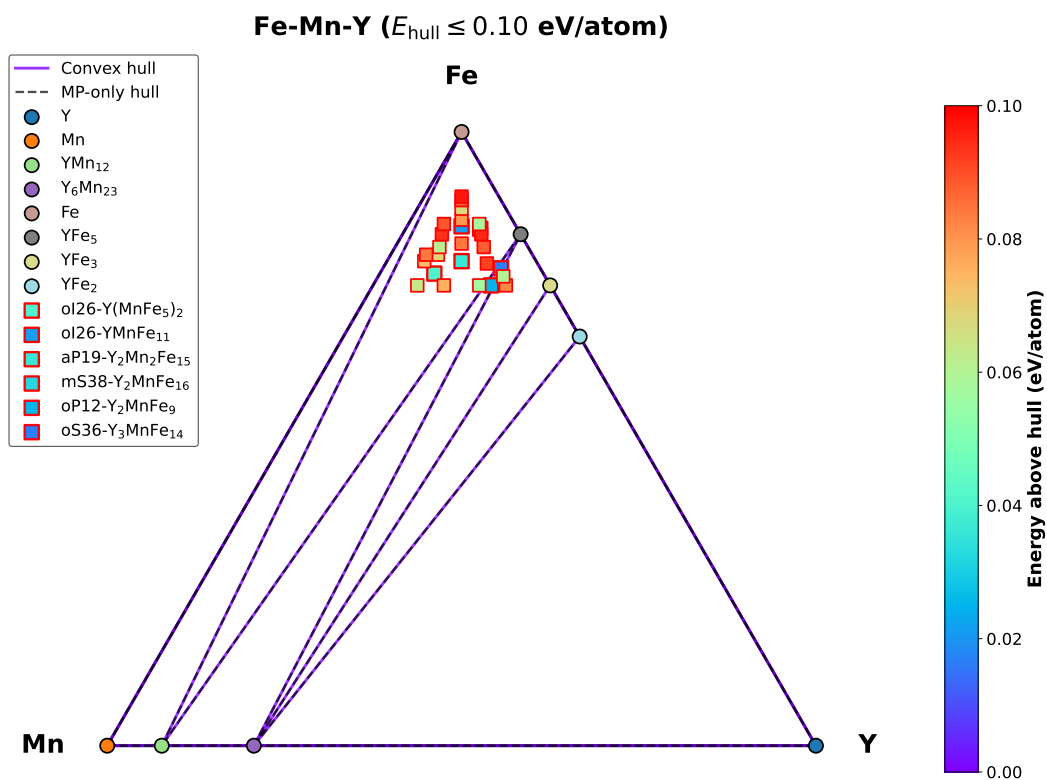


Figure S15: Ternary hull for the Fe–Mn–Y system.

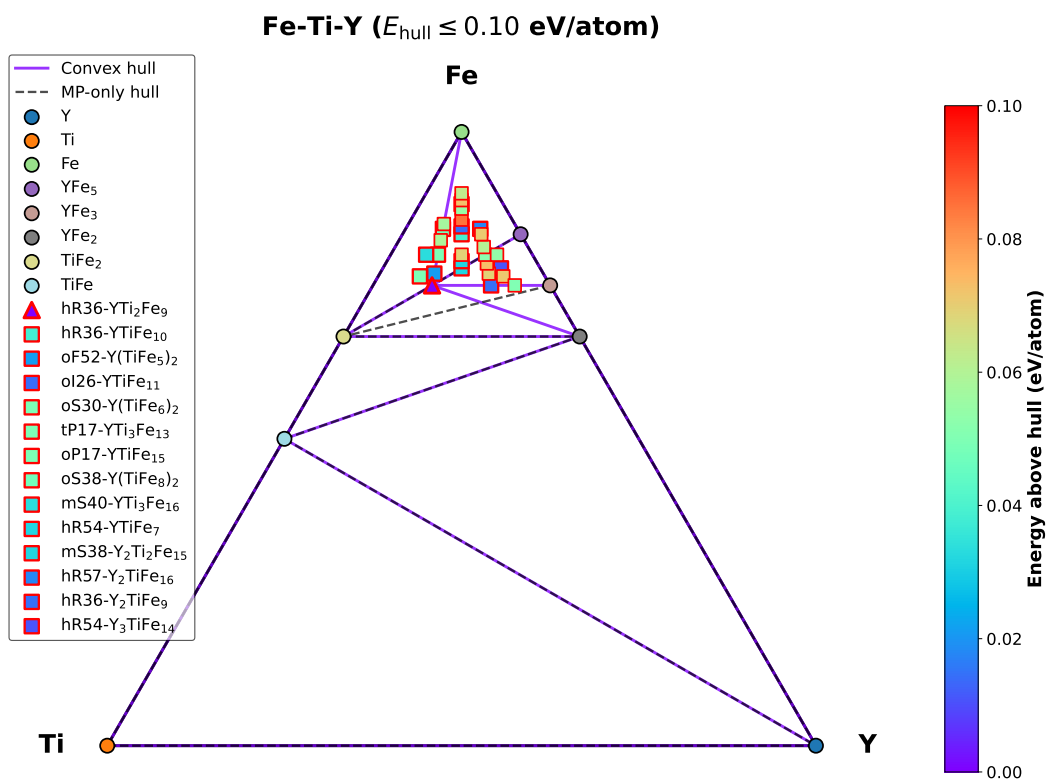


Figure S16: Ternary hull for the Fe-Ti-Y system.

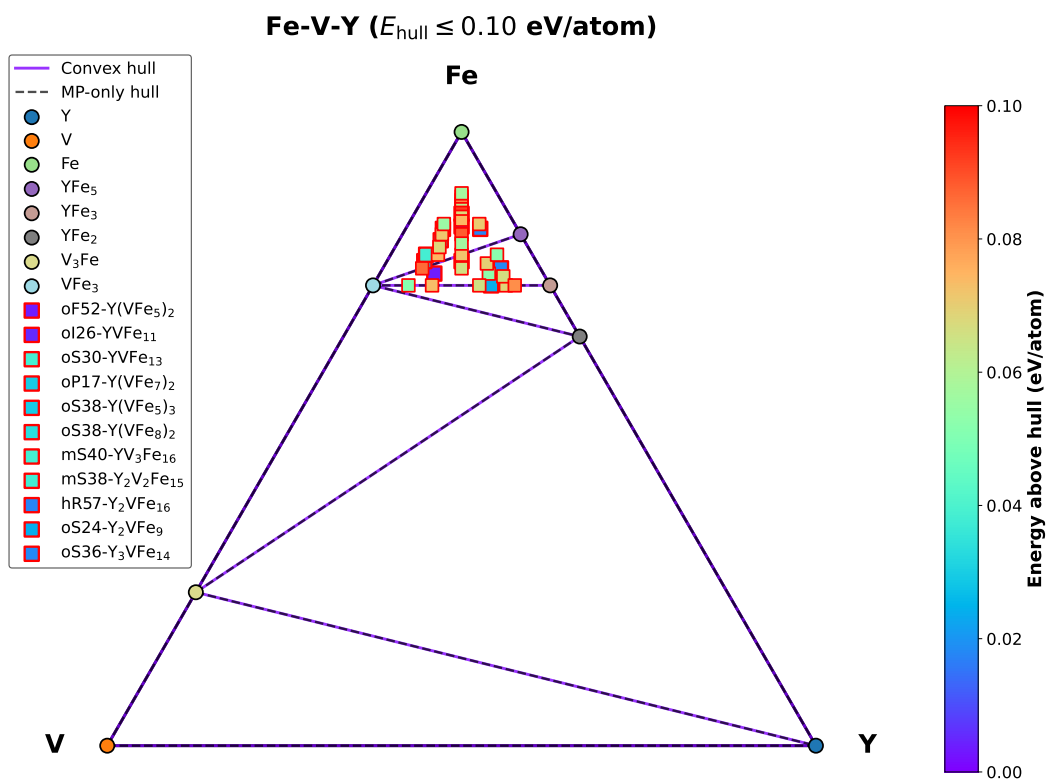


Figure S17: Ternary hull for the Fe–V–Y system.

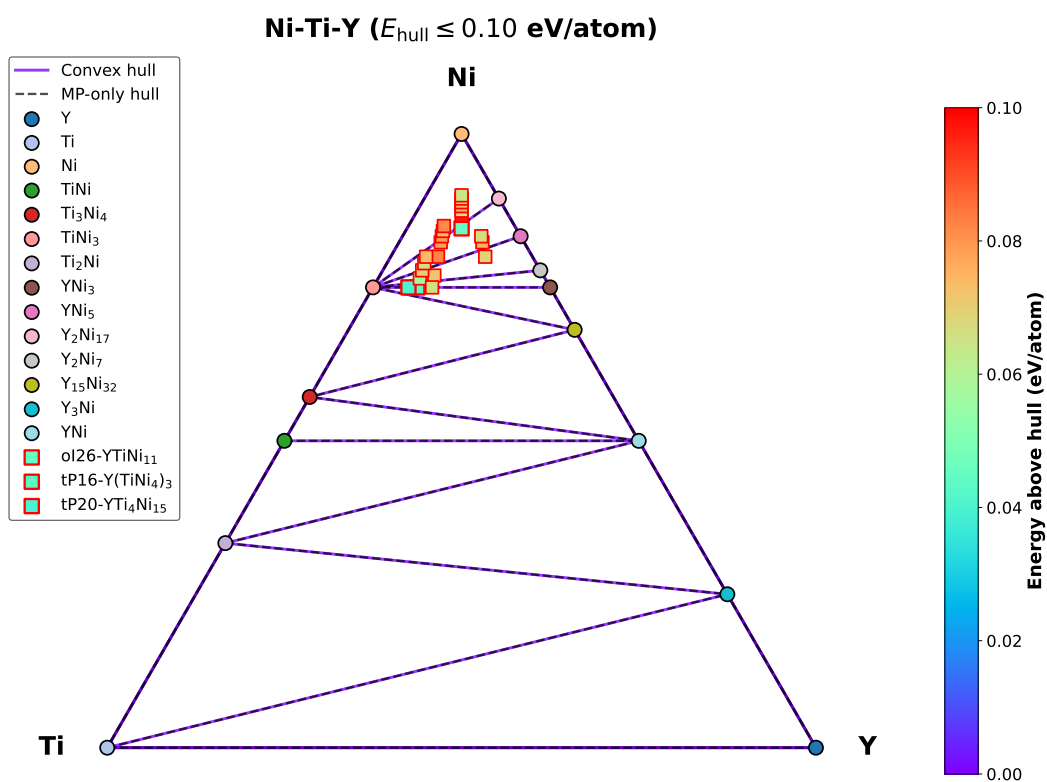


Figure S18: Ternary hull for the Ni-Ti-Y system.

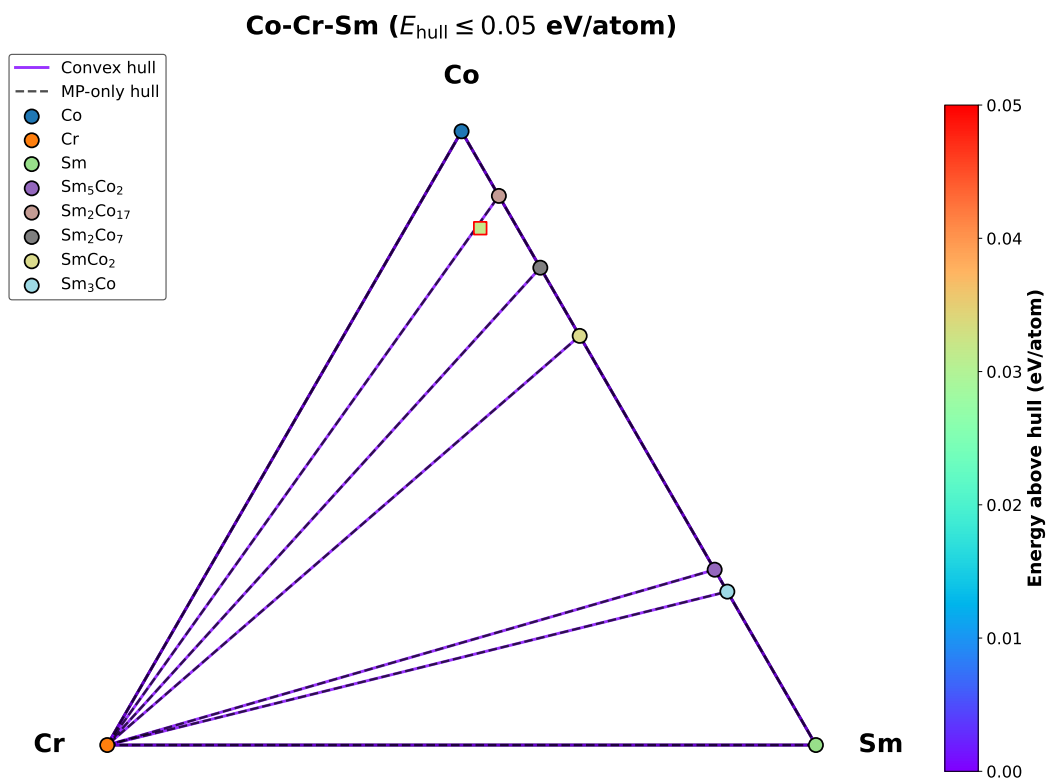


Figure S19: Ternary hull for the Co–Cr–Sm system.

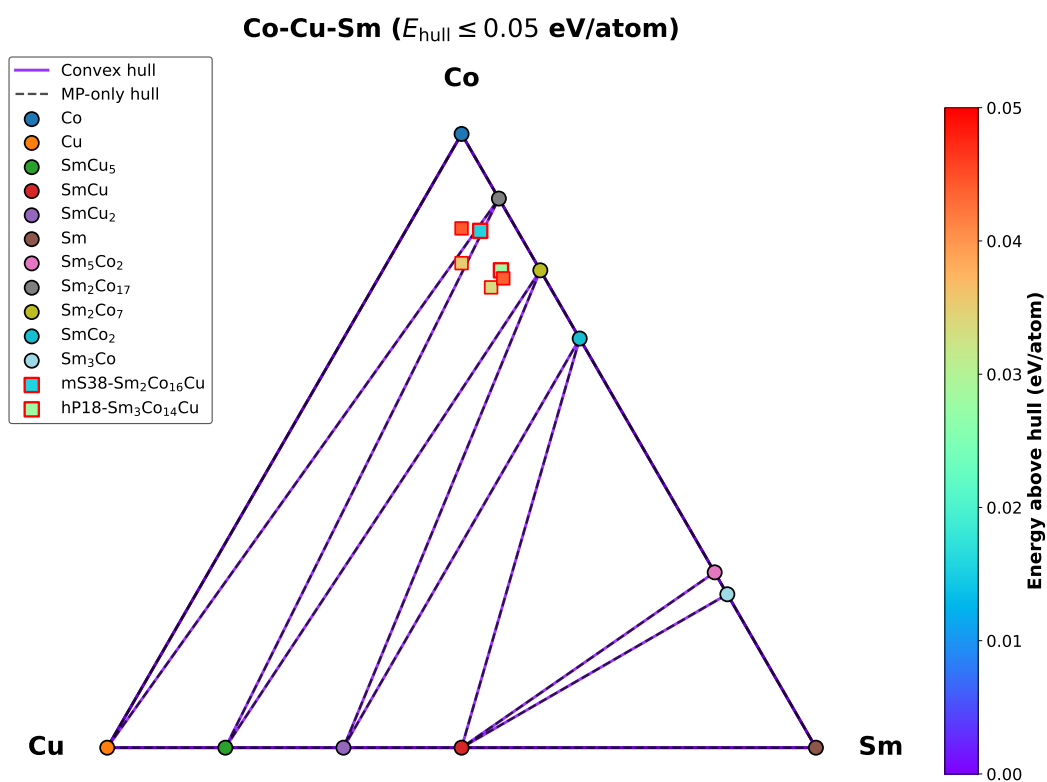


Figure S20: Ternary hull for the Co–Cu–Sm system.

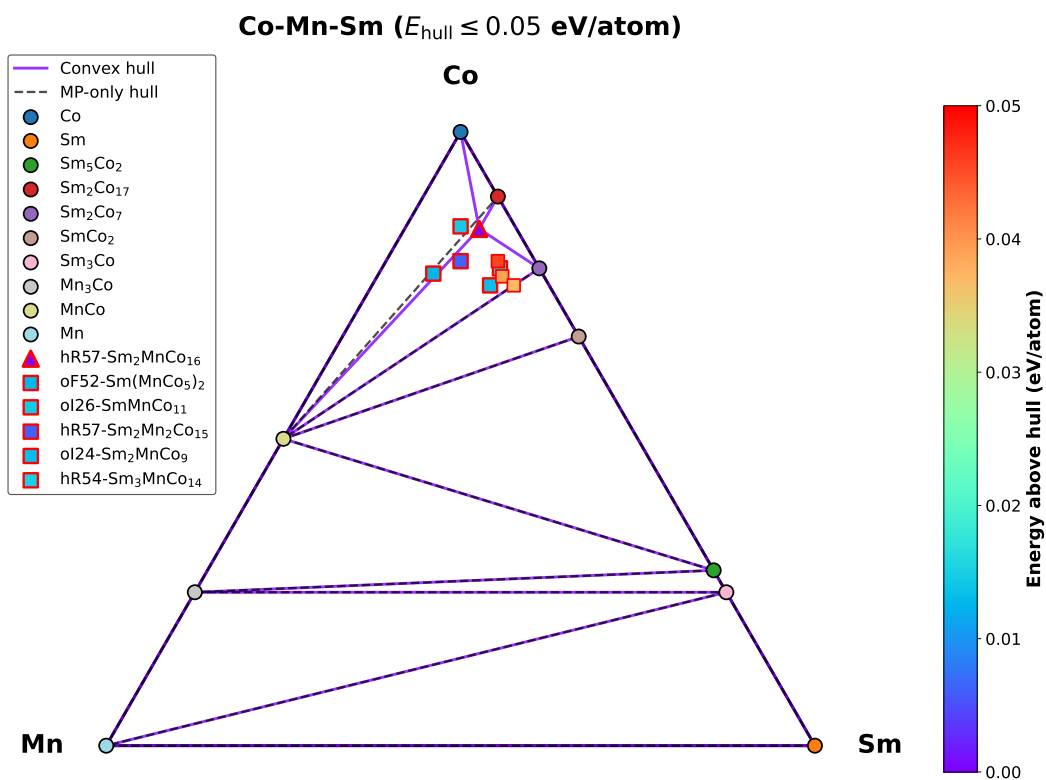


Figure S21: Ternary hull for the Co–Mn–Sm system.

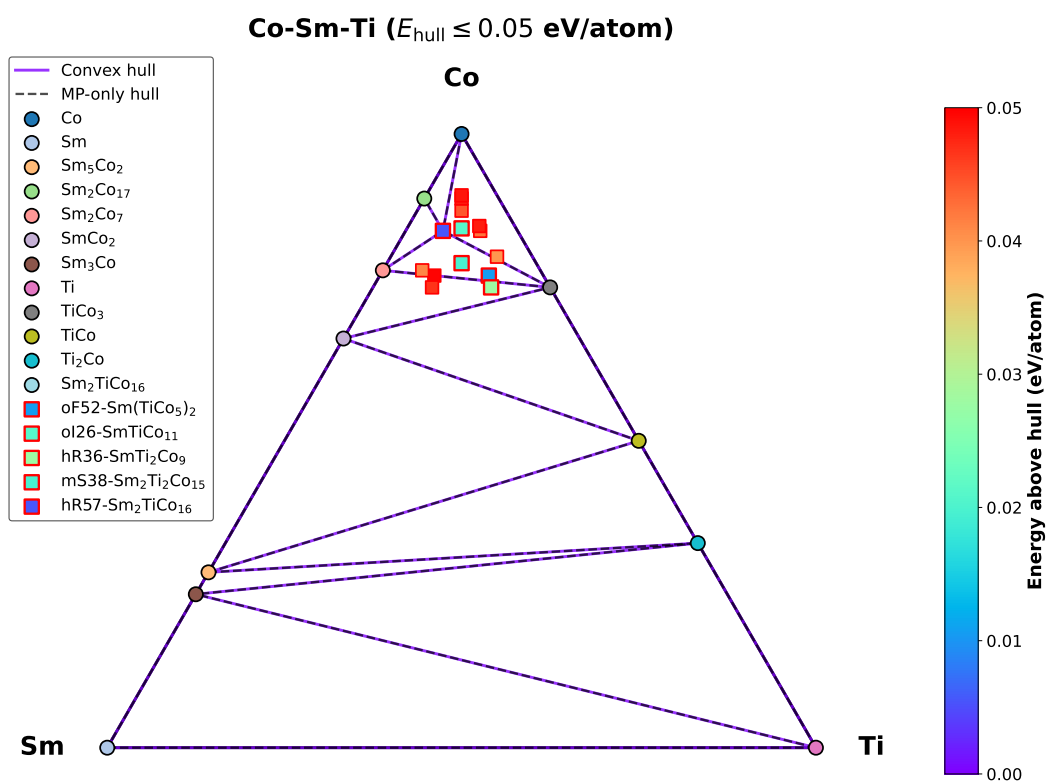


Figure S22: Ternary hull for the Co-Sm-Ti system.

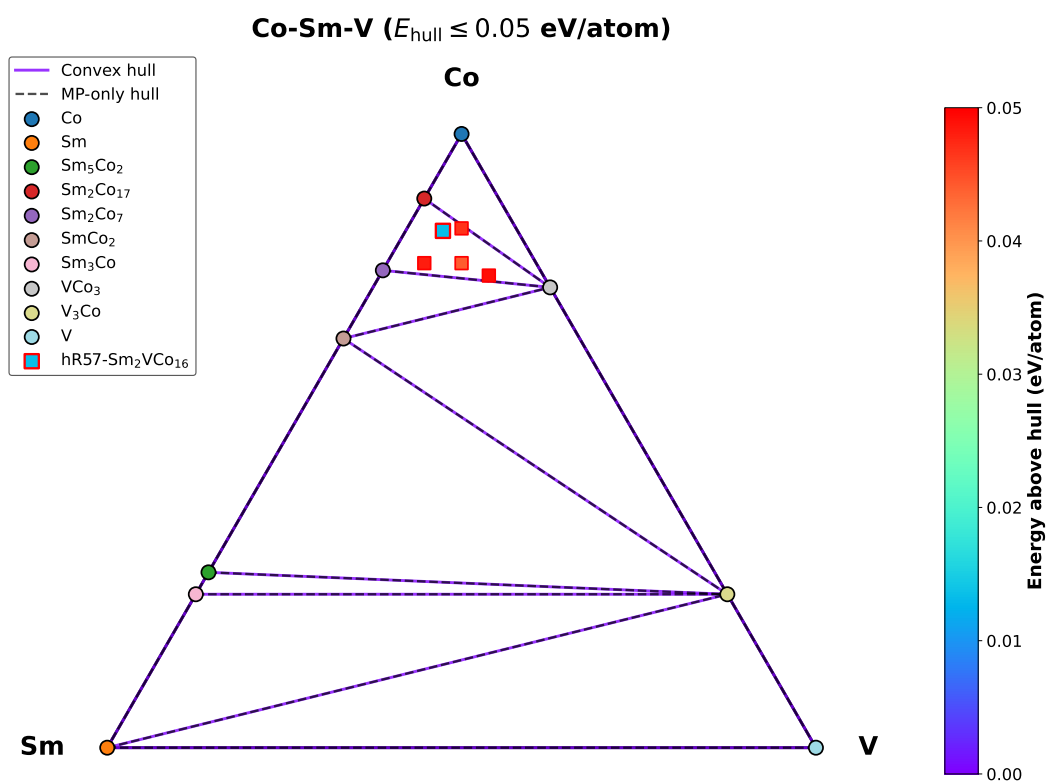


Figure S23: Ternary hull for the Co-Sm-V system.

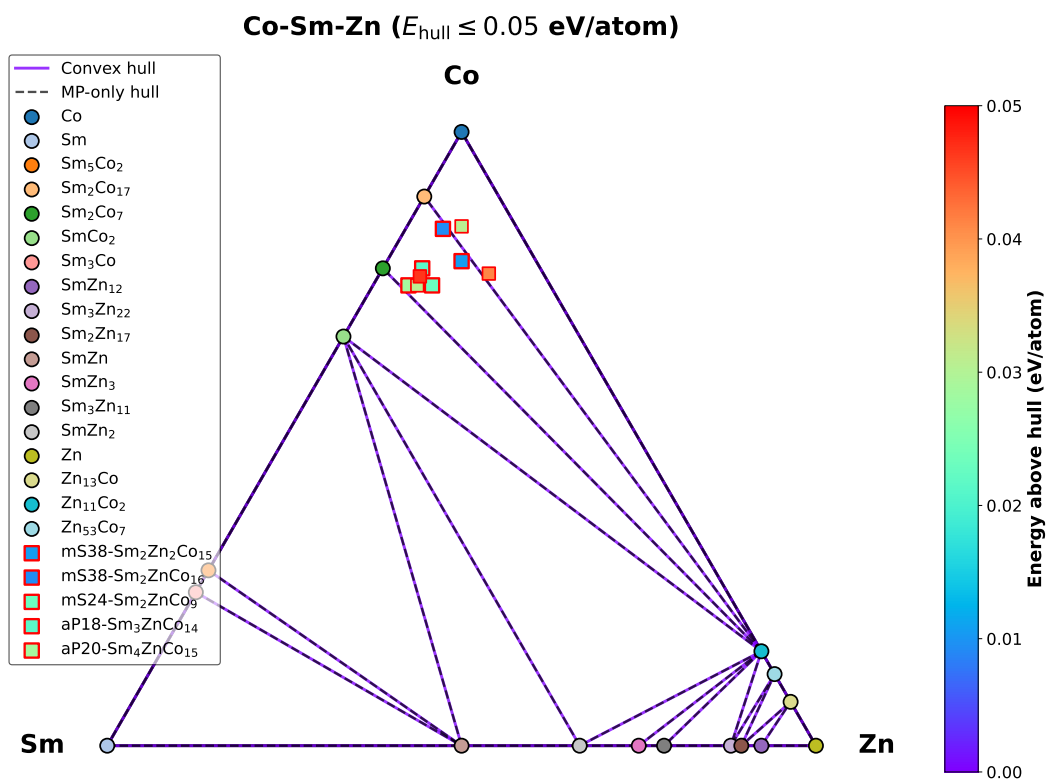


Figure S24: Ternary hull for the Co–Sm–Zn system.

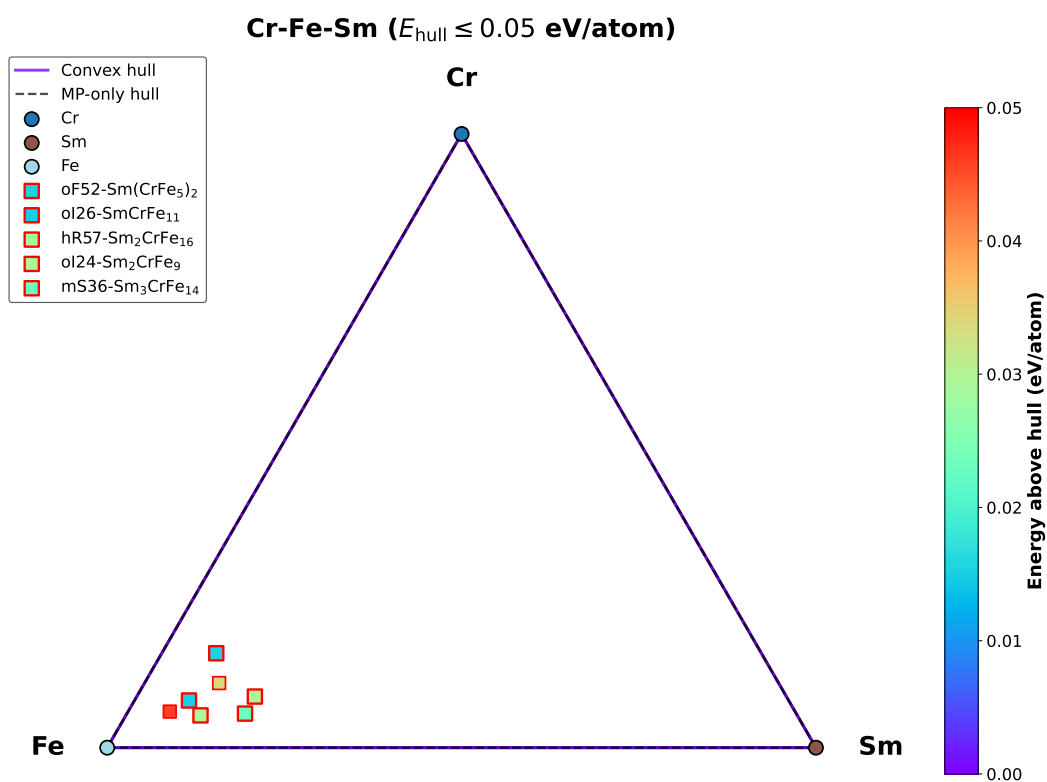


Figure S25: Ternary hull for the Cr–Fe–Sm system.

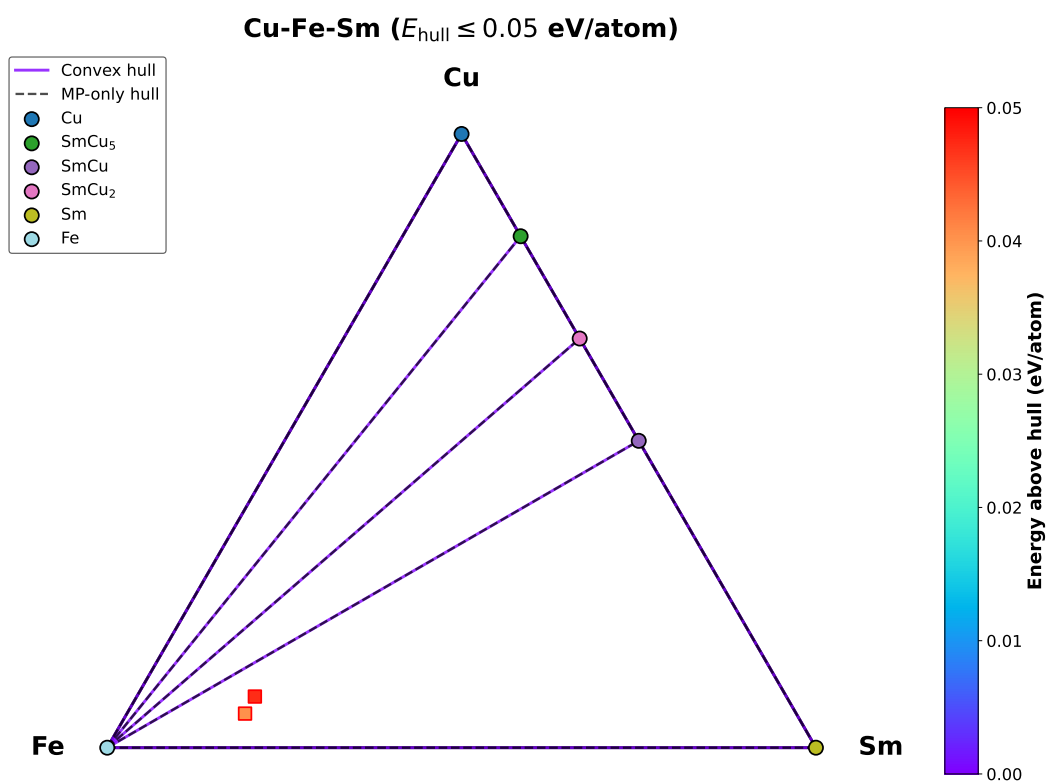


Figure S26: Ternary hull for the Cu-Fe-Sm system.

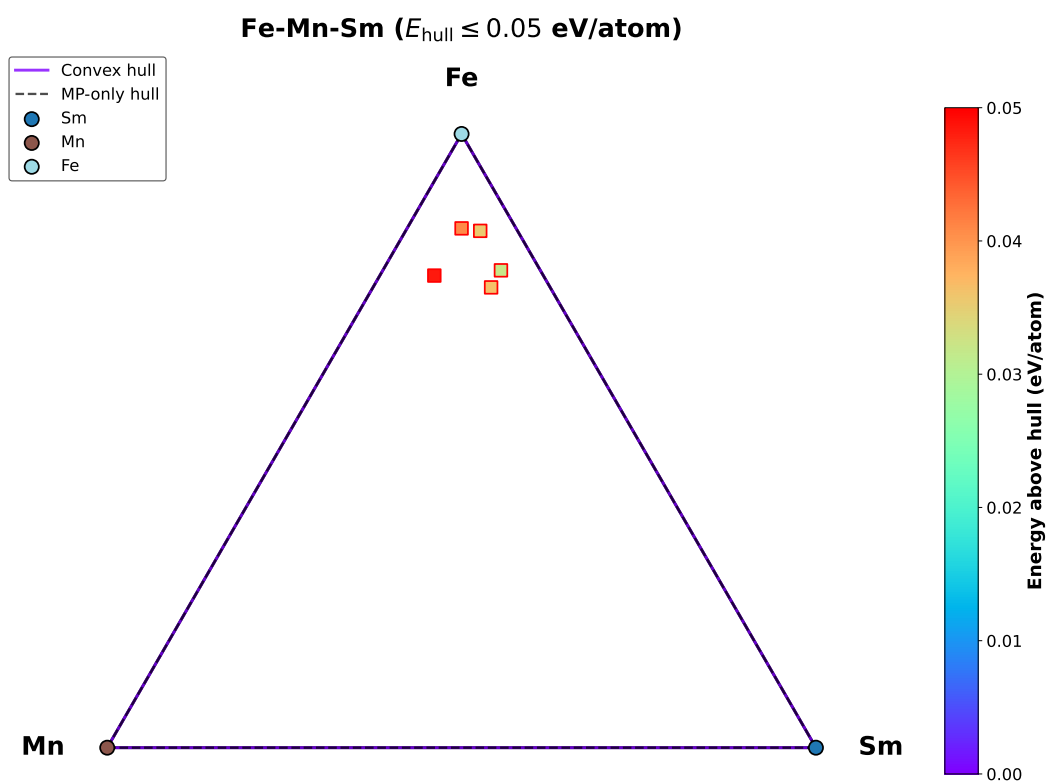


Figure S27: Ternary hull for the Fe–Mn–Sm system.

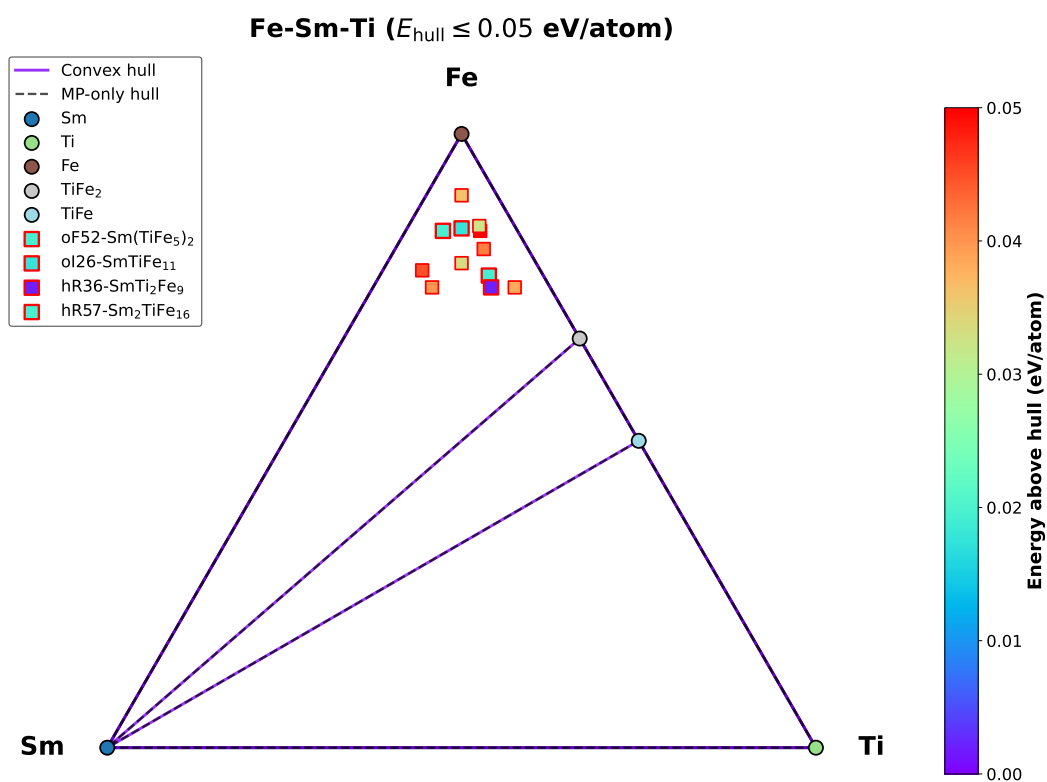


Figure S28: Ternary hull for the Fe-Sm-Ti system.

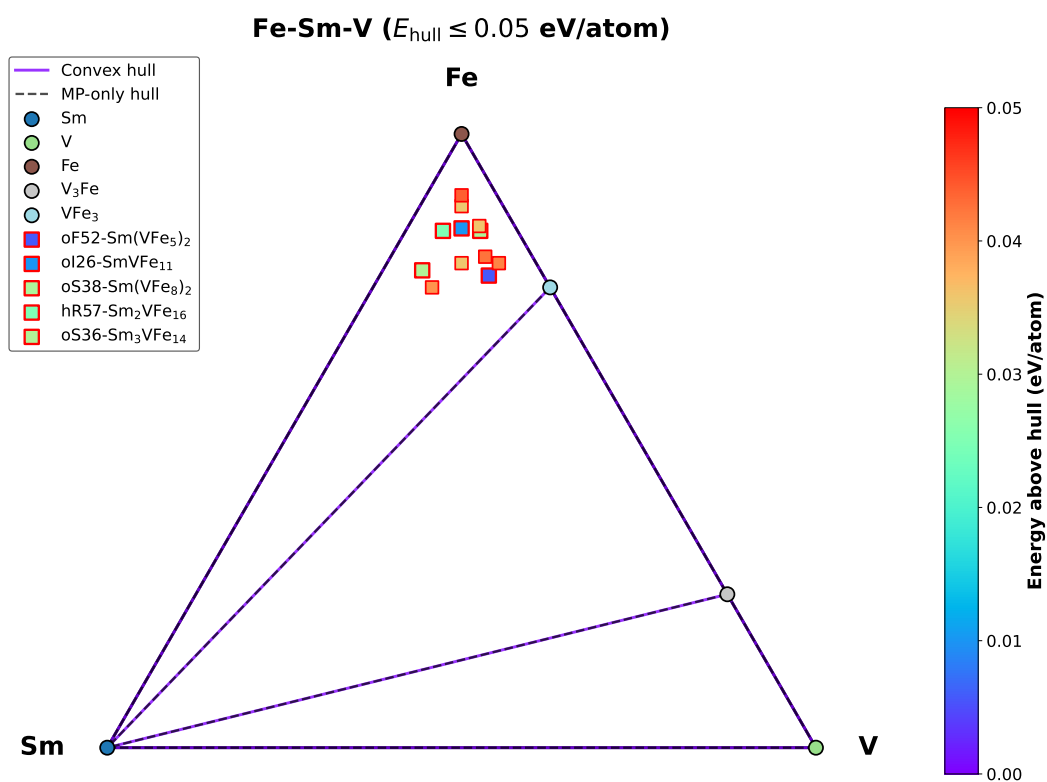


Figure S29: Ternary hull for the Fe-Sm-V system.

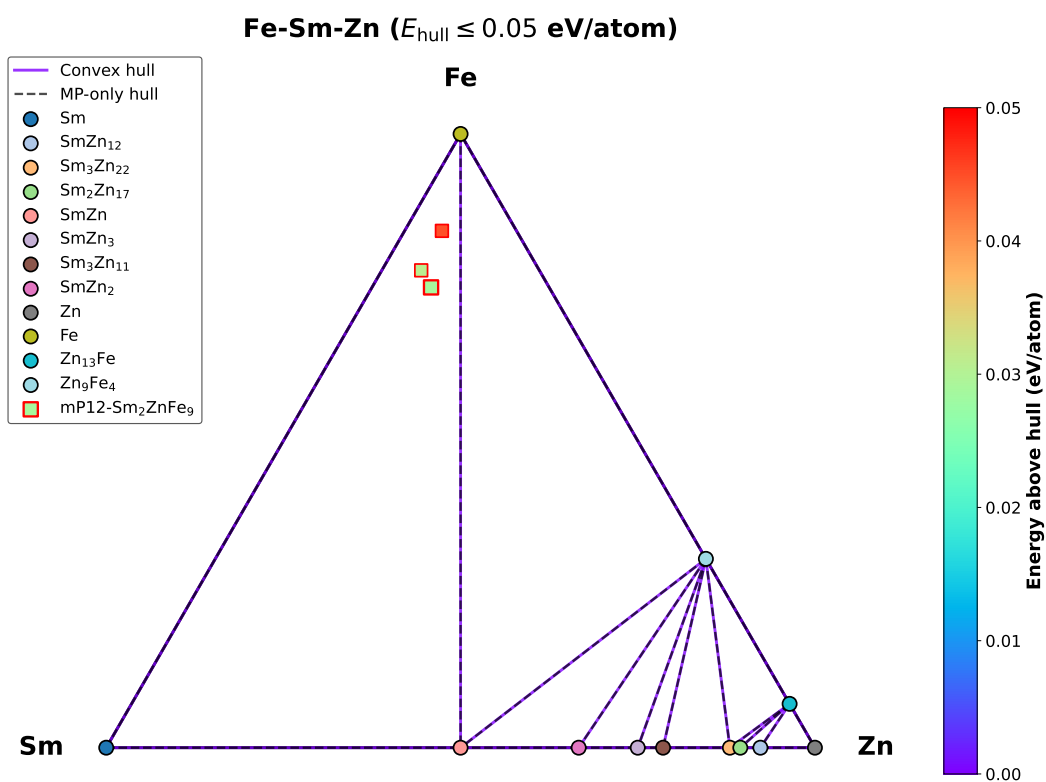


Figure S30: Ternary hull for the Fe–Sm–Zn system.

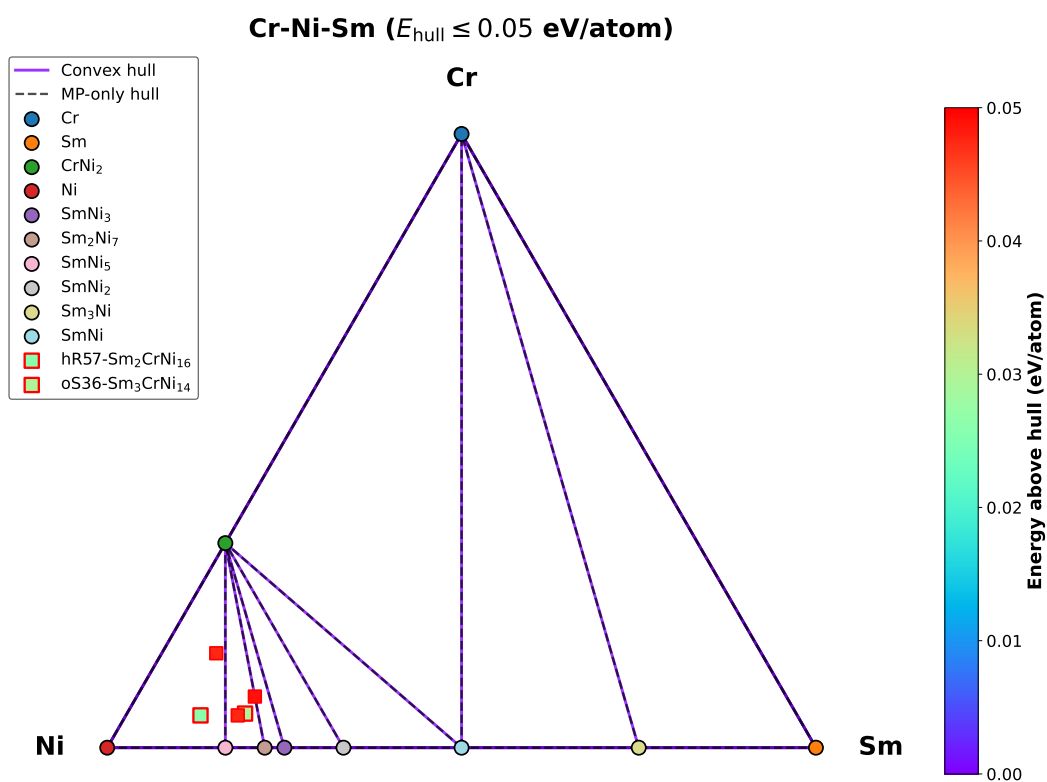


Figure S31: Ternary hull for the Cr–Ni–Sm system.

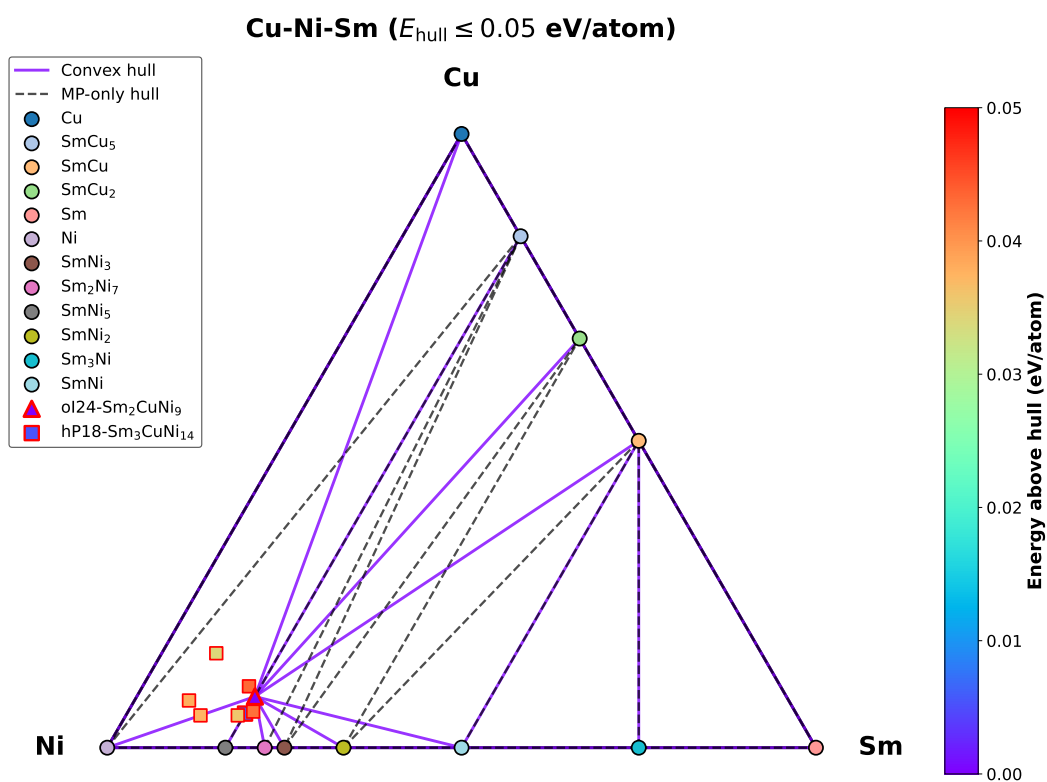


Figure S32: Ternary hull for the Cu–Ni–Sm system.

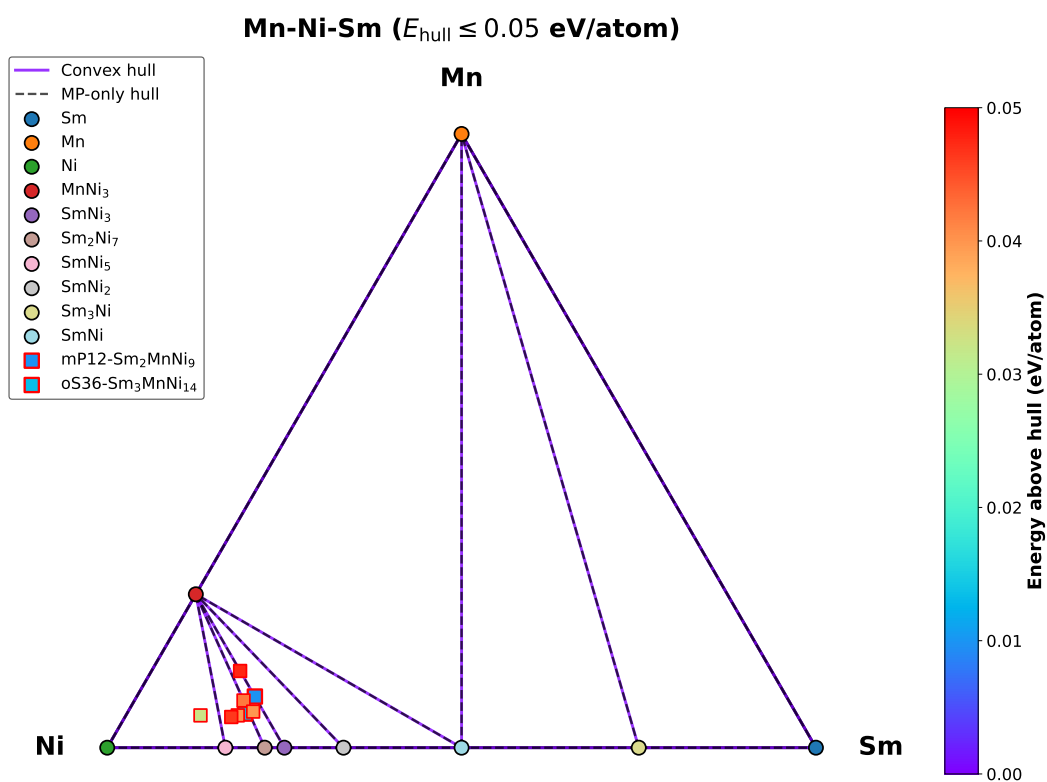


Figure S33: Ternary hull for the Mn–Ni–Sm system.

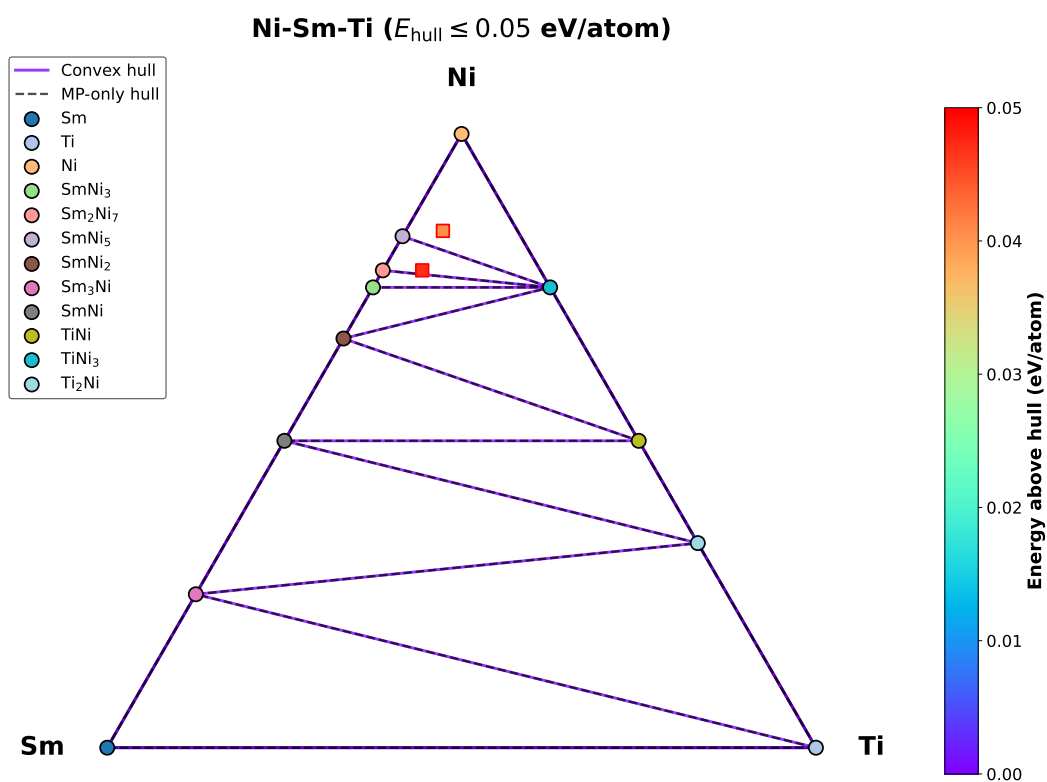


Figure S34: Ternary hull for the Ni-Sm-Ti system.

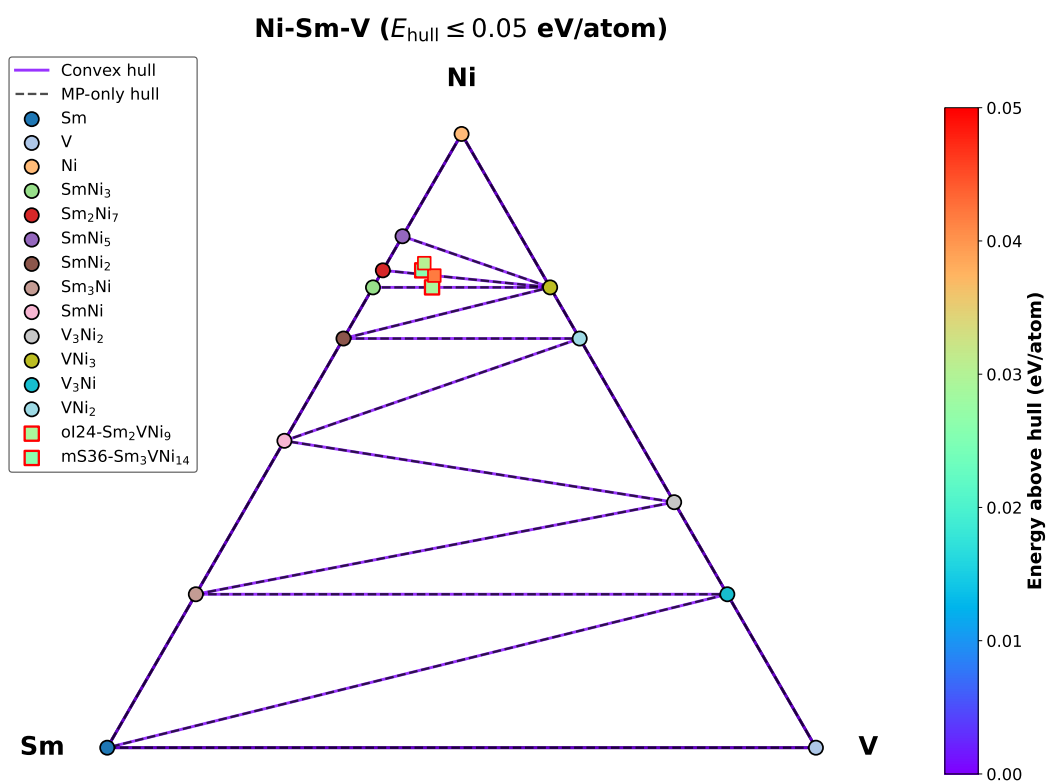


Figure S35: Ternary hull for the Ni-Sm-V system.

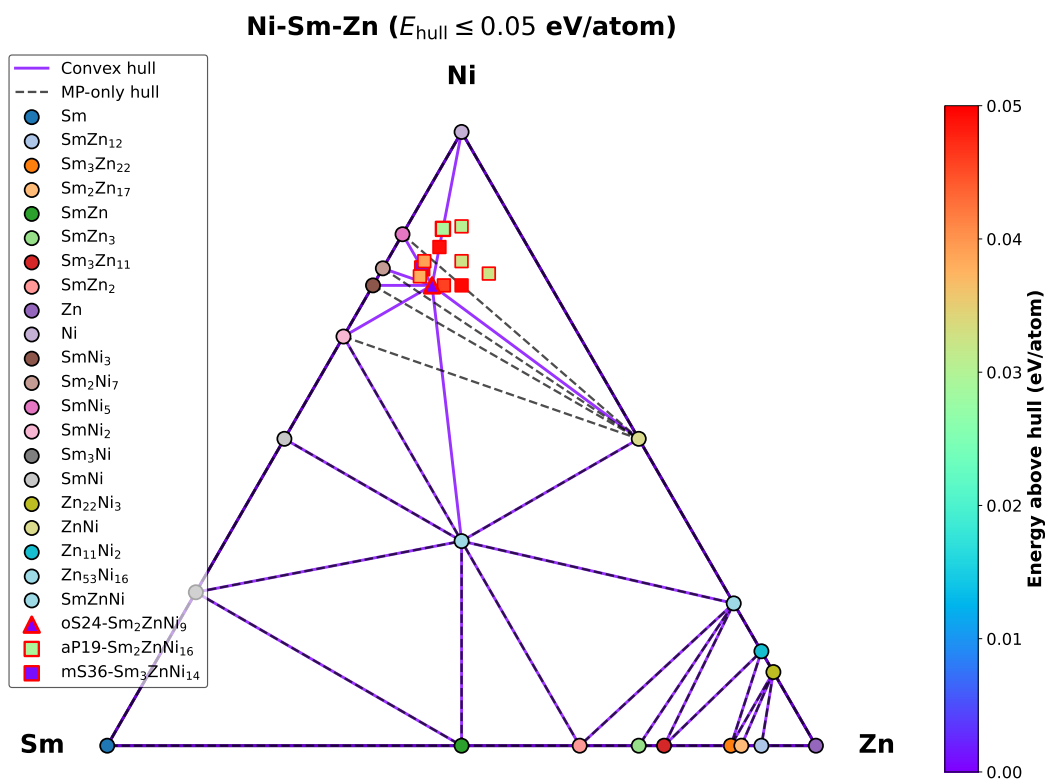


Figure S36: Ternary hull for the Ni-Sm-Zn system.