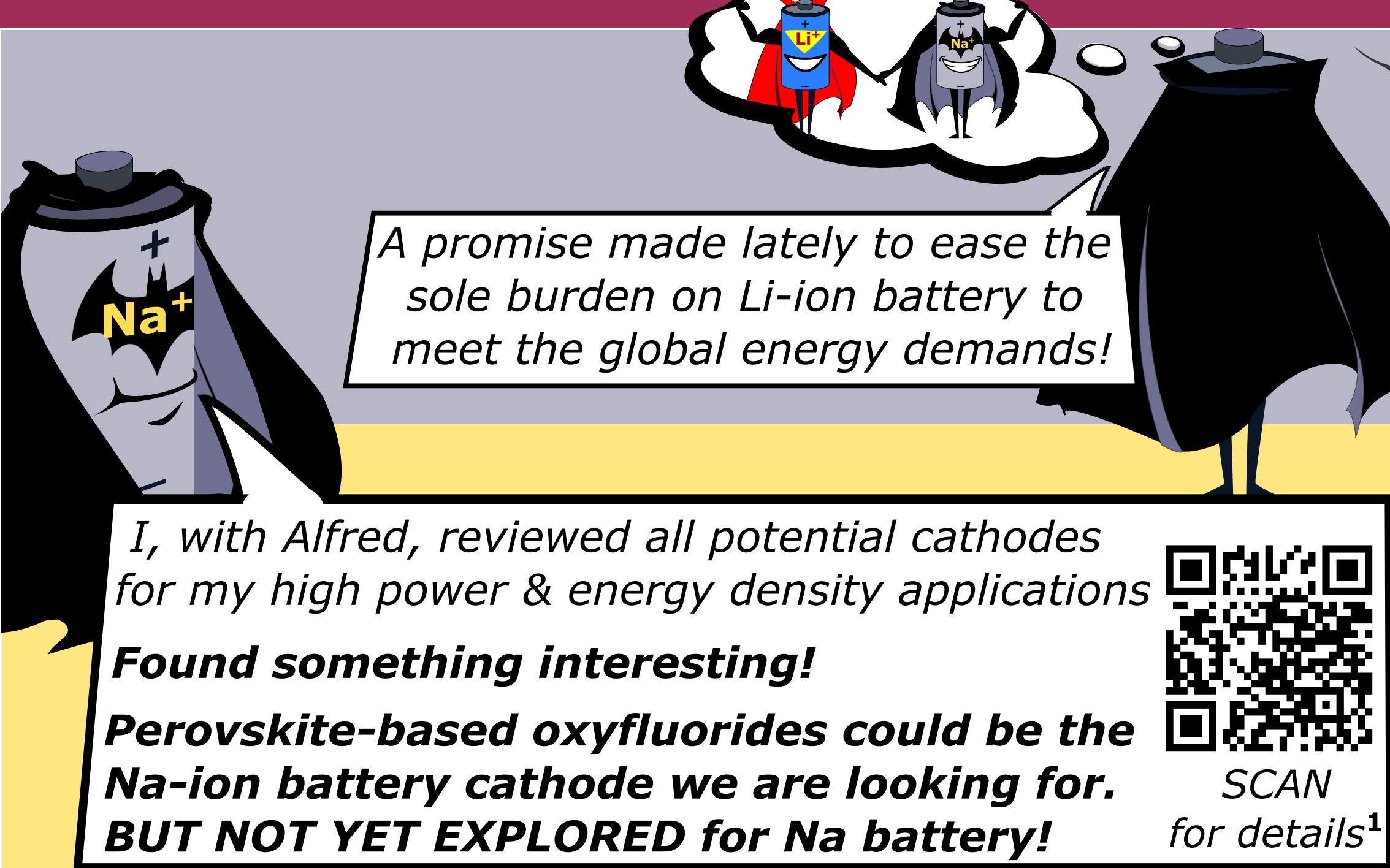


Exploration of polyanionic fluoride-based compounds as Na-ion battery cathodes

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WHY PEROVSKITE OXYFLUORIDES?

I. General formula: $\text{Na}_x\text{MO}_{3-y}\text{F}_y$, where, x= Na content, M= 3d transition metal, y= F content

II. Perovskites: Ideal framework for big-sized Na-ion insertion

III. Highly electronegative F elevates voltage by inductive effect; Light-weight O-F anionic group raises specific capacity

Synthesis difficulty from highly stable fluoride precursors limited perovskite-oxyfluoride research as battery cathode²

Tried a few oxyfluorides as cathode for myself; TiOF_2 ($Pm\bar{3}m$)³ & VO_2F ($R\bar{3}c$)⁴ amorphised during cycle while $\text{Li}_2\text{MO}_2\text{F}$ ⁵ have disordered rocksalt framework.

Good Li-ion mobility though!⁶ Wanna Try?

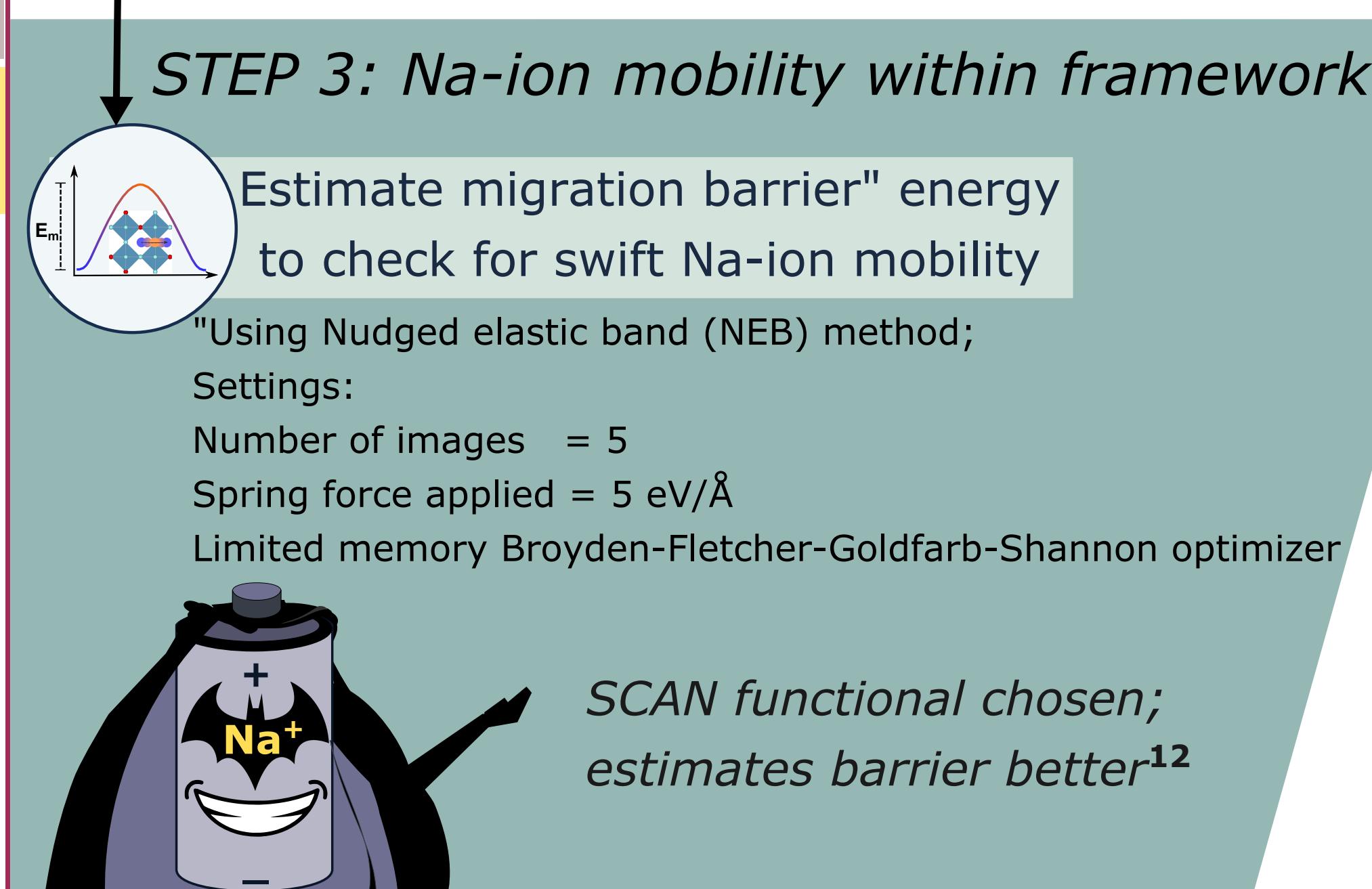
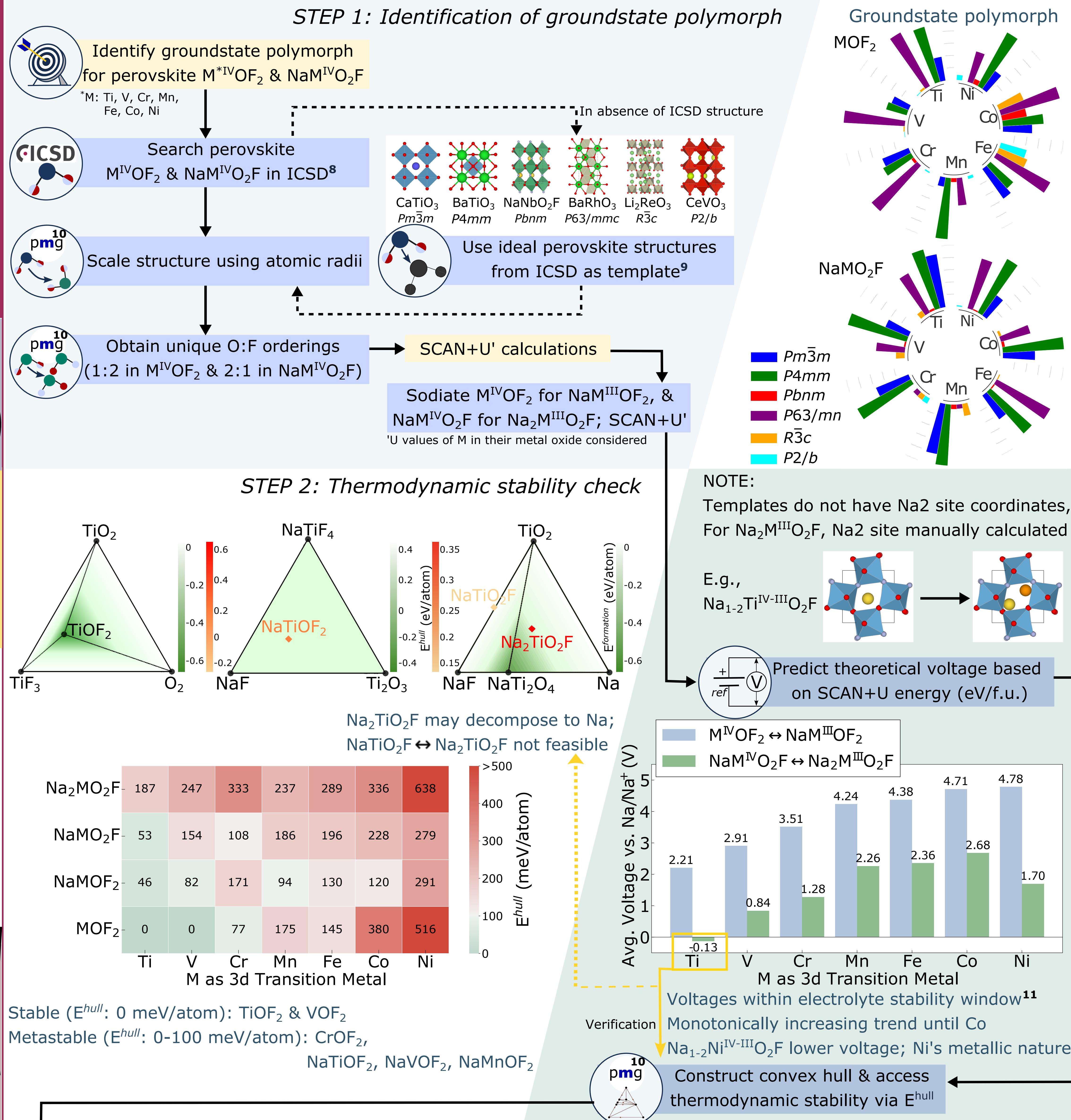
Not sure about Na-ion mobility in amorphised/disordered structure.⁷ Na^+
Gotta begin with crystalline ordered perovskite oxyfluoride!

$\text{Na}_{0-1}\text{M}^{IV-III}\text{OF}_2$ & $\text{Na}_{1-2}\text{M}^{IV-III}\text{O}_2\text{F}$ chosen stoichiometry

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METHODOLOGY & OBSERVATIONS



We are not so far from discovering perovskite-based oxyfluorides as potential cathodes.
Stay tuned!



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WORK IN PROGRESS

NEB with SCAN calculations are ongoing for thermodynamically stable & metastable compositions

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