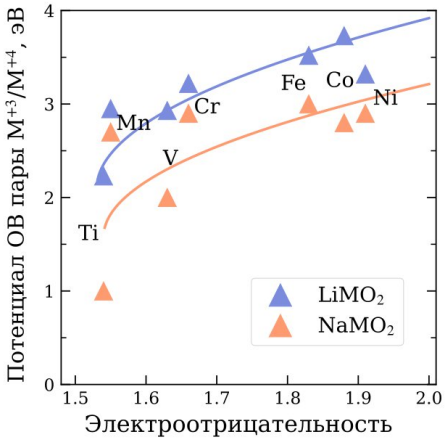
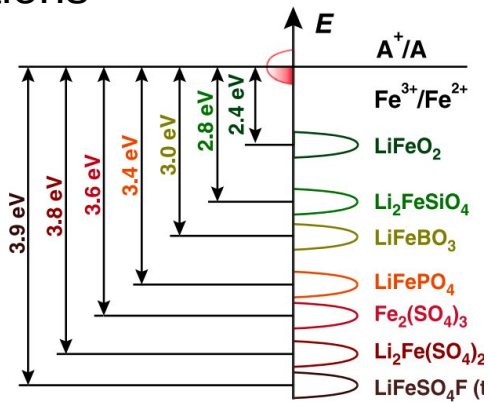
Task 1 for group 1: Effect of TM on redox potential

- Take $NaNiPO_4$ (mp-776388)
- Replace transition metal (M) by V, Fe, Mn, Co
- Optimize their lattice constants ($NaMPO_4$)
- Remove all the Na atoms to get composition MPO_4
- Optimize their lattice constants (MPO_4)
- Calculate volume changes and intercalation potentials $NaMPO_4/MPO_4$
- Plot dependence Intercalation Potential from Electronegativity of TM



Task 1 for group 2: Effect of Ligand on redox potential

- Find structures of Na_xNi-L, L = PO_4, BO_3, SO_4, SiO_4 in Materials Project database and in the literature
- Optimize their lattice constants
- Remove all the Na atoms to get deintercalated compositions
- Optimize their lattice constants
- Calculate volume changes and intercalation potentials
- Plot dependence Intercalation Potential (Ligand type)



Task 2

- Take SEI composition from Table in Slide 4
- Find in literature what crystal structure it has [use Materials project]
- Optimize its lattice constants
- Construct a supercell - no more than 30-40 atoms
- Calculate migration barrier of LI for all possible directions

SEI for the projects

Material and MP entry	Number of atoms	Space group	Supercell size in units and A	Number of atoms in a big cell
NaF (682)	8	Cubic	3x3x3 (11x11x12 A)	54
Na_2O (2352)	12	Cubic	2x2x2 (8x8x8 A)	24
Na_2SO_3 (21282)	12	Trigonal	2x2x1 (11x11x6 A)	48
Na_2SO_4 (4770)	56	Orthotombic	1x1x1 (6x9x12 A)	56
NaClO3 (23330)	20	Cubic	1x1x1 (7x7x7x A)	20

References:
1-4: https://onlinelibrary.wiley.com/doi/epdf/10.1002/aenm.202002297
5: https://pubs.rsc.org/en/content/articlepdf/2020/cc/c9cc08221b