Functional Materials Design and Discovery Using Bayesian Optimization

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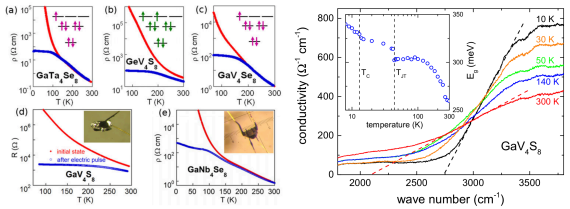
Academic Disciplines:
MATERIALS SCIENCE & ENGINEERING
MECHANICAL ENGINEERING

June 13, 2019

Motivation

Metal-insulator transition (MIT) material $AM_1M'_3Q_8$
(A=Al,Ga,In; M,M'=V,Nb,Ta,Cr,Mo,W; Q=S,Se,Te)



Understanding composition-property relationship

- how different elements influence material properties, e.g. metallicity, magnetism, polarization

Designing controllable MIT materials

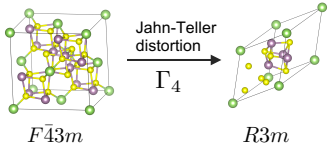
- High resistive switching ratio
- Stable at ambient conditions

Reschke, et.al. *Phys. Rev. B* **96**, 144302 (2017)
Corraze, et.al. *Eur. Phys. J. Special Topics* **222**, 1407-1056 (2013)

Design Objectives

- **Maximizing band gap (E_g):** **Better functionality**

Hypothesis:
Larger band gap
↓ Structural distortion
Higher resistive switching ratio

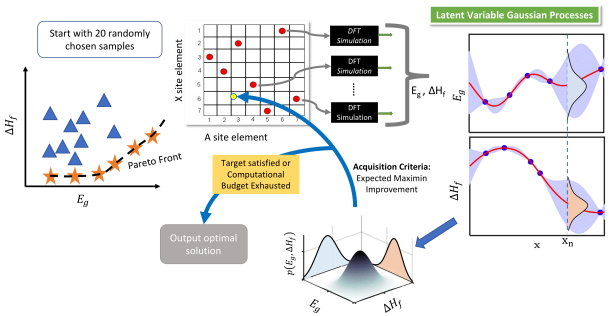


- **Minimizing formation energy (ΔH_f):** **Higher stability**

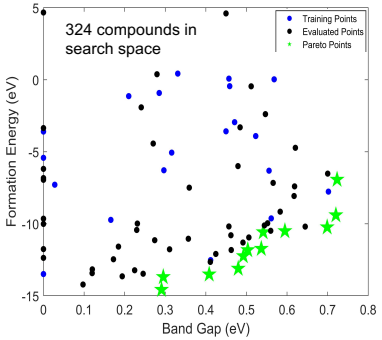
$$Ga + Mo + 3 * Cr + 8 * S \rightarrow GaMoCr_3S_8$$

$$\Delta H_{rxn} = \sum \nu \Delta_f H(product) - \sum \nu \Delta_f H(reactant)$$
$$= \Delta_f H(GaMoCr_3S_8) - \Delta_f H(Ga) - \Delta_f H(Mo) - 3 * \Delta_f H(Cr) - 8 * \Delta_f H(S)$$

Multi-objective Bayesian Optimization



Exploring the Pareto front



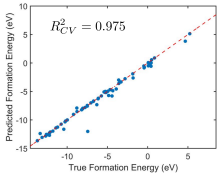
Discovered 6 out of 9 compounds on the Pareto front within 60 iterations

Computationally efficient

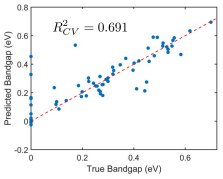
Validating model accuracy

5-fold cross validation

- ❑ Highly-accurate in formation energy prediction
  - Easier to learn additive patterns



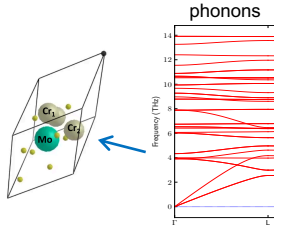
- ❑ Performance less ideal for band gap prediction
  - More materials info needed



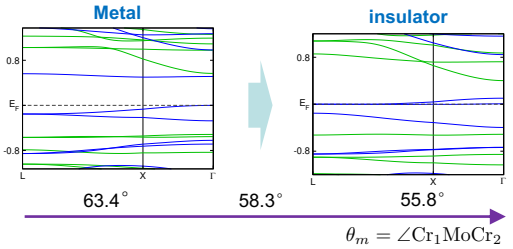
Materials by Design

Novel MIT compound $Ga_1Mo_1Cr_3S_8$

Low-frequency phonon mode corresponding to the cluster distortion



Simulating the metal-insulator transition



More candidate MIT materials

- $Al_1V_1Nb_3S_8$
- $Al_1V_4S_8$
- $Al_1V_1Ta_3S_8$
- $Al_1Cr_1V_3S_8$
- $In_1Mo_1Ta_3S_8$
- $Al_1Ta_1V_3S_8$
- $Ga_1W_1Cr_3S_8$

Conclusions

- ❖ Developed an effective way to search the composition space of lacunar spinel family
- ❖ Performed multi-objective Bayesian optimization and successfully obtained 9 compounds on the Pareto front
- ❖ Used DFT to simulate the metal-insulator transition and validated our hypothesis

Northwestern University