Using Density Functional Theory to Predict the Formation Energies of AI/ML Generated Superconducting Structures

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Introduction

JOHNS HOPKINS APPLIED PHYSICS LABORATORY

The Applied Physics Laboratory (APL) at Johns Hopkins University (JHU) is programming an AI/ML algorithm that can generate potential superconducting structures (PSS).
The project is to utilize Density Functional Theory (DFT) to calculate the formation energies of these PSS and feed the data gathered back into the algorithm.

QUANTUMESPRESSO

The DFT Package used is "Quantum Espresso," which is a free open-source software containing several pseudo-potentials.
The functional type used was the Perdew-Burke-Ernzerhof Generalized Gradient Approximation (PBE-GGA) for all structures.

The Materials Project

All crystal structures, except for the PSS, where DFT calculations were performed on are all from "The Materials Project."

Project

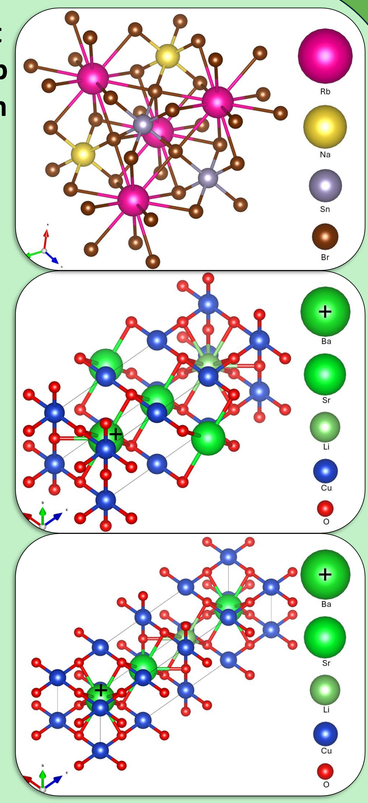
DFT calculations were done on multiple PSS, with most calculations not completing do to the unorthodox setup of the crystal structures. The focus of this poster is from the top to bottom:

$Rb_2NaSnBr_6$
$BaSrLiCu_3O_5$
$BaSr_2LiCu_4O_7$

Where the calculations were able to complete.

$$\frac{\Sigma E_F \text{ Prod} - \Sigma E_F \text{ Reag}}{\Sigma \text{Atoms of Superconductor}}$$

A stoichiometry equation is set up with a PSS being one of the products, along with the relevant reagents and extra products. The formation energy of the PSS is then calculated using the equation above where the difference of the sum of formation energies of the products and the sum of formation energies of the reagents, divide it by the sum of atoms of the current PSS. If the formation energies equals a positive, DFT predicts the PSS will not form, and if negative, DFT predicts the PSS might form. Data is then compared to experimental data.



PSS	Reagent	PSS + Product	E_f
$BaSrLiCu_3O_5$	$Ba + Sr + Li + Cu_3 + O_5$	$BaSrLiCu_3O_5$	-
$BaSrLiCu_3O_5$	$2BaCO_3 + 2SrOC_3 + Li_2CO_3 + 6CuO$	$2BaSrLiCu_3O_5 + 5CO_2 + \frac{1}{2}O_2$	+
$BaSr_2LiCu_4O_7$	$Ba + Sr_2 + Li + Cu_4 + O_7$	$BaSr_2LiCu_4O_7$	-
$BaSr_2LiCu_4O_7$	$2BaCO_3 + 4SrCO_3 + Li_2CO_3 + 8CuO$	$2BaSr_2LiCu_4O_7 + 7CO_2 + \frac{1}{2}O_2$	+
$Rb_2NaSnBr_6$	$Rb_2 + Na + Sn + Br_6$	$Rb_2NaSnBr_6$	-
$Rb_2NaSnBr_6$	$2RbBr + NaBr + SnBr2 + Br$	$Rb_2NaSnBr_6$	-
$Rb_2NaSnBr_6$	$2RbBr + Na + SnBr_4$	$Rb_2NaSnBr_6$	-
$Rb_2NaSnBr_6$	$2RbBr_3 + Na + Sn$	$Rb_2NaSnBr_6$	-
$Rb_2NaSnBr_6$	$4RbBr + 2NaBr + SnBr_2 + SnBr_4$	$2Rb_2NaSnBr_6$	+

- All structures are energetically favorable when reagents are the elements
- $BaSrLiCu_3O_5$ and $BaSr_2LiCu_4O_7$ are not energetically favorable when reagents are the carbonates (carbon-oxide) and oxides
- $Rb_2NaSnBr_6$ was tested for Multiple reactions
  - Was shown to be energetically favorable until all relevant elements were in compound form

Conclusion

Given the predictions of the calculations, this could indicate that the PSS the AI/ML algorithm generates are likely not possible because compound-based reagents that are typically used in synthesis, especially considering the cuprates (copper-oxygen), are not coming out as energetically favorable. A potential explanation is due to the PSS not existing, therefore, the DFT calculations are predicting a positive energetic favorably as so. Further investigation is necessary as the calculations can be implemented differently in QE as well as the data being compared to more experimental data.
What is shown is that DFT can models different reactions to better guide the experimentalists on synthesis. Given the many PSS generated by the AI/ML algorithm rejected, many DFT calculations not completing (mostly being the cuprates), and the lack of energetically favorable reactions with the PSS that do complete in the DFT calculation, the APL AI/ML algorithm has much development to undergo. Ultimately, there are numerous amounts of PSS that are worth looking into. The data found during this project will be fed back into the algorithm which will then improve the accuracy.

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