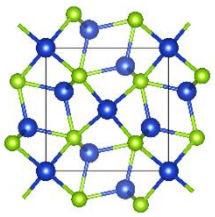
You are invited to attend a lecture on

DATA-BASED ASSISTED THEORETICAL PREDICTION OF CHALCOGENIDE MATERIALS



Alon Hever

Ph.D. student under the guidance of Dr. Amir Natan

Thursday, February 10, 2021, at 15:00

Join Zoom Meeting

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Abstract

Mapping all possible materials and their properties is the ultimate goal of material sciences. Beyond the purely scientific interest, discovering new materials with unique properties leads to improved technologies that can change our life—computational material science helps to fulfill these goals by predicting such materials. Identifying new stable or metastable structures with a sensible computational cost requires an intelligent selection of structures out of an astronomical number of atoms arrangement possibilities. In this talk, I show a compound discovery method assisted by data analysis of the most extensive database for crystalline materials, the inorganic crystal structure database (ICSD). In the first part, we will see the statistics of ICSD's binary and ternary chalcogenide (O, S, and Se) compounds. This analysis found a relatively high overlap between binary sulfides and selenides structure types but also found that some stoichiometries and structures which exist in one family are missing from the other. We, therefore, assumed that structure types of binary sulfides could enrich binary selenides and vice versa to find new stable compounds[1]. In the second part, we apply this structure types enrichment approach for eight binary systems of sulfides (A_xS_y, A = Bi, Ti, Cu, and Nb) and selenide (A_xSe_y, A = Cu, Ta, Zr, and As) by substituting the Se atom with S and the other way around. A second strategy for structure enrichment included structures that came from $\tilde{A}S$ and $\tilde{A}Se$ compounds whose $\tilde{A}$ atom arrives from the same or neighbor column of the periodic table as the A element in AS and ASe. Finally, A third strategy for enrichment was to select all the possible $\tilde{A}_xS_y$, $\tilde{A}_xS_y$, $\tilde{A}_xSe_y$ structure types only for the Ti_xS_y, Cu_xS_y, and Ta_xSe_y families, where now $\tilde{A}$ could be from any place on the periodic table. The structures from the three strategies led to the finding of twelve new compounds compared to the known ICSD's structures, where ten structures came from neighbor column compounds, one came from a second neighbor column, and one from Lanthanides elements. The discovery rate using the neighbor methods was, on average, one new compound for every twenty structures that were tested. This indicates a simple and effective heuristic method for finding new compounds that can be easily applied in other systems[2].

1. Hever A., Oses, C. Curtarolo, S., Levy, O. & Natan, A. The Structure and Composition Statistics of 6A Binary and Ternary Crystalline Materials. *Inorg. Chem.* **57**, 653–667 (2017).

2. Hever A., Levy O. & Natan A. Directed search for new chalcogenide compounds based on composition and structure analysis. In preparation