Computer design of new electrolytes for solid-state batteries

Chepkasov I V[@], Maltsev A P and Oganov A R

Skolkovo Institute of Science and Technology, Skolkovo Innovation Center Bldg 3, Moscow 143026, Russia

[@] I.Chepkasov@skoltech.ru

We aim to find all stable phases in the specified systems (Li-O-F, Li-O-Cl, Li-O-Br, Li-O-B, Li-O-I, Li-S-F, Li-S-Cl, Li-S-Br, Li-S-I, Li-O-S-F, Li-O-S-Cl, Li-O-S-Br, Li-O-S-I, Li-P-S, Na-P-S, K-P-S)– and if possible also low-energy metastable ones. All of these systems are very complex and it is tempting to use data mining as a cheap method, but its use has to be benchmarked. As an alternative, much more expensive and reliable USPEX searches can be used. We used two most famous databases—Materials Project(MP) and OQMD. To find out which phrases are stable, we combined the data from Material Database and OQMD and built a joint convex hull using our USPEX-code. Comparing the results from the two databases, we found many differences. For example in Li-B-H we found large differences between MP and OQMD: in MP we see phases LiB, BH_3, B_2H_5, B_5H_7 and B_9H_{11}, which are not seen in OQMD (which sees instead $B_{10}H_{13}$ and B_9H_{11} as stable. To search new compounds of phase with Li we used the USPEX code. All required compositions were considered. For each composition we calculated no less than 20 generations, each generation of 300 new configurations. Several new phases have been found.

Conclusion

1.Neither of the popular data mining approaches, Materials Project and OQMD, gives a correct and complete phase diagram for our systems of interest.

2.The use of USPEX allows you to find a large number of phases, both already known and completely new.

We acknowledge funding from Russian Science Foundation (grant No. 22-73-00219)