Prediction of new materials for solid-state batteries

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We aim to find all stable phases in the specified systems (Li-P-S, Na-P-S, K-P-S, Li-Ge-S, Na-Ge-S, K-Ge-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 Na-P-S we found differences between MP and OQMD: in MP we see structure NaP7, which are not seen in OQMD (which sees instead N4P3 and NaP5 as stable). To search new compounds of phase we used the USPEX code. Each subsequent generation consisting of 300 structures was produced by applying the heredity (40% of each generation), softmutation (20%), and transmutation (20%) operators; 20% of each generation was produced using random symmetric and random topological structure generators.These calculations allowed to find the most suitable materials for solid-state batteries.

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 the Russian Science Foundation (project No. 22-73-00219)