## MS18-P19 | COMBINATION OF DATA MINING AND DFT MODELING OF $Ag^+$-CONDUCTIVITY IN S(SE)-CONTAINING INORGANIC COMPOUNDS

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Now the Li-batteries meet problems of large-scale production: they are unsafe and expensive due to depletion of natural resources. Replacement of the Li conductors with new high-conductive substances is a great challenge for materials science. One of the solutions is the processing of large amounts of structural data to mine prospective ion conductors. We use fast database screening by means of ToposPro program package [1], which we have designed for modeling of ion conductivity. We have adopted Voronoi approach to explore $Ag^+$-ion migration in S(Se)-containing compounds and selected 826 ternary and quaternary Ag and S(Se)-containing compounds from the last ICSD. The 91 S- and 42 Se-containing structures were found, which possess 1D, 2D or 3D $Ag^+$-ion migration maps.

Out of them, 87 compounds have not been examined before as $Ag^+$-ion conductors and can be recommended for experimental testing. Further, we estimated the migration energies for 13 compounds by the NEB method within the DFT approach and found a good agreement with the experimental conductivity for $Ag_4P_2S_6$, $AgCrS_2$ and $Ag_3PS_4$. Such combination of fast crystallochemical and precise DFT methods can serve as an effective prediction scheme to search for new fast-ion conductors.

[1] Vladislav Blatov, Alexander Shevchenko, Davide Proserpio //*Cryst. Growth Des.* 2014. V. 14.7. P. 3576-3586.