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Ionic conductors based on metal-closo-borates

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Solid state compounds with ionic conductivity larger than 1 mS/cm at room temperature can compete with liquid electrolytes when applied in rechargeable batteries. Recently new sulfide materials with this property were discovered, extending family of ionic conductors based on oxides.

Very high conductivity of sodium reported in $\text{Na}_2\text{B}_{12}\text{H}_{12}$ competes with the best solid state conductors known for this metal. Further developments brought borane based Na superionic conductors that are by orders of magnitude better than those based on β -alumina.

We will present theoretical study, based on DFT calculations, explaining the conductivity mechanism in closo-borates, as well as pointing out the differences in conductivity of lithium and sodium.

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