The dependence of the proton conductivity on concentration for networks with different symmetry of molecules

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ABSTRACT

The proton conductivity in solids is carried out mainly by the Grotthuss mechanism, a two stage mechanism of proton migration consisting of thermally induced reorientation of molecules and proton hopping between minima of the hydrogen-bond potential [1].

A model of conducting path may be realized by a chain of rods or other objects depending on the symmetry of molecules taking place in the reorientation. Rods are sufficient to represent flips of heterocyclic molecules in the case of heterocyclic based polymers [2]. For the solid acids built form tetrahedral molecules triangles instead of rods are needed while for the perovskites squares as a representation of octahedra.

The conductivity in the one dimensional chain of rods reveals substantial fall for the concentration of protons equal to 0.5 [2]. This behaviour was explained using symmetry arguments and recognized as a geometrical blocking. We show that for the chain of triangles also a strong decrease of conductivity is presented for the concentration 0.5 but in addition it is observed in a wide range of concentration around 0.5. Since for triangles the geometrical blocking cannot be the explanation of the downfall thus the analysis of sources for this is presented.

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References

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