

## Vibrational properties of closo –borane anions in superionic conductors

*Wednesday, 11 September 2019 09:00 (20 minutes)*

Metal closo-borate compounds have attracted recent attention as superionic lithium or sodium conductors. In  $\text{Na}_2\text{B}_{12}\text{H}_{12}$  or  $\text{Li}_2\text{B}_{12}\text{H}_{12}$  the superionic phases are related to the temperature induced phase transitions [1]. Modification of the crystal structure or ion substitution provide the means of tuning their cation conductivity. Spectroscopic fingerprint of internal closo anion ( $\text{B}_{12}\text{H}_{12}^-$ ) vibrations provides unique opportunity to study influence of such modification in the crystal properties. Dynamical fingerprint of anion vibrations is related to the nature of cation –anion interactions.

We report on theoretical calculations of the change of IR and Raman modes of  $\text{B}_{12}\text{H}_{12}$  structure upon deformation along the high symmetry axes as well as interaction of such anion with model configuration of cations. These anions are aromatic structures and even smallest deformations are related to changes in B –H stretching frequencies of entire structure. Deformation is related to change of the electronic structure that extends over whole anion. Our systematic studies of anion dynamical properties are confronted with experimental evidence of Raman modes and cation conductivity.

### Summary

### Topic

1. Theoretical and experimental methods

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