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Bonding states of Cu atoms in superionic α-CuI phase HIROAKI OSHIHARA, KAZUO TSUMURAYA, Meiji University, Japan — The fast migration of cations in solids is used for solid state battery. Therefore the mechanism of the migration is of importance for the development new material. The superionic conductor CuI is zinc blend-type structure at low temperature and fluorite-type at high temperature. So the bonding between Cu and I atoms has been considered to be a covalent bonding. The peak positions and the asymmetrical peaks in the pair distribution functions between the Cu-Cu and Cu-I components have been remained to be explained in an experiment and a computational studies. We investigate the electronic states of CuI using the planewave based density functional calculation. We evaluate the charge and bonding states with Bader decomposition method. The stability of the Cu-Cu pairs in the conductor will be discussed using their binding energies.

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