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Charge and Bonding States of Ag Atoms in Superionic Conductor α-AgI MASATO ITO, KAZUO TSUMURAYA, Meiji University, Japan — The fast migration mechanism of the cations in the superionic conductors has been little known up to now. In the case of α-AgI, the charge states of the Ag atoms and the bonding states between Ag and I atoms during the migration remain to be explained. No explanation has also been given for the origin of both the positions and the asymmetric first peaks of the Ag-I and Ag-Ag pair distribution functions. We investigate the electronic states of AgI using the first principles electronic structure calculations. We use the Bader analysis to evaluate the charges that belong to each atom and obtain the ionicity of the atoms. The stability of the cation pairs in the conductor will be discussed using their binding energies.

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