Why are the copper cations superionic in the $\alpha$-CuI crystal?
KAZUO TSUMURAYA, TAKAMITSU OHTSUKA, HIDEKAZU TOMONO, Meiji University — The mechanism of the superionic conduction is an unresolved issue in the solid-state physics. The cations are mobile species in $\alpha$-CuI and $\alpha$-AgI crystals. In these conductors, the constituent atoms are ionized. The clarification of the mechanism of the high mobility of the cations needs to investigate the electronic structures in the $\alpha$-CuI crystal. We obtain the dynamically-averaged local (DAL) positions of the mobile copper cations in the crystal from the pair distribution function and the angle distribution functions, which we calculate from the first principles molecular dynamics simulations at 700 K. The positions predict the existence of a correlation among the cations in the $\alpha$-CuI. The static electronic structure analysis, of the DAL structure, allows us to clarify the correlation. The correlation enables us to clarify the mechanism of the migration and the difference in the electronic structures between the conductors and the ionic crystals.