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Electronic properties and mechanism of superionic conductivity in Li_3N MASARU AOKI, Shizuoka Sangyo University, KAZUO TSUMURAYA, Meiji University — Lithium nitride is a superionic conductor with high Li conductivity. The compound has been studied intensively because of its potential utility as electrolyte in solid-state batteries. Though it is known that the charge carriers responsible for conduction are Li vacancies in the Li_2N plane, the mechanism of the high mobility remains unsolved. To clarify the origin of the mobility we simulate the dynamics in the Li_3N crystal with the first principles molecular dynamics method. We have found the existence of the cooperative dynamics of Li ions in the Li_2N plane.

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