論文の内容の要旨

Theoretical Study on Electron States Floating in Internal Space of Condensed Matter Based on First-Principle Calculations

（第一原理計算に立脚した凝縮物質の内包空間に広がる電子状態の研究）

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I report first-principles electronic-structure calculations that clarify the floating nature of electron states in covalent semiconductors. It is found that wave functions of several conduction- and valence-band states, including the conduction-band minima, do not distribute near atomic sites, as was taken for granted, but float in interstitial channels in most semiconductors. The floating states have a nearly-free-electron (NFE) like character, and extend in the channels broadly without atomic-orbital characters. The electrostatic potential at the channels and the directions and shapes of the interstitial channels depend on the crystal symmetry so that mysterious variation of the energy gaps in silicon carbide (SiC) polytypes is naturally explained by considering the floating nature.

The substantial band-gap variation in SiC has been analyzed by an empirical parameter ”hexagonality” for a half century. Yet, I have clarified that the parameter ”hexagonality” is a misleading parameter. Instead, I have found that a new parameter channel length, which represents the spatial extension of the floating state, is essential in describing the band-gap variation in SiC. In addition, I have performed the linear-combination-of- atomic-orbitals (LCAO) calculations and compared the results with those calculated by the plane-wave-basis set. It is found that the floating characters in the

electron states are difficult to find in the LCAO calculations. We also examined the floating states in pressurized sp^3-bonded materials. We have also found that the energy bands consisting of floating states manifest different behavior from other bands consisting of atomic orbitals under the pressurized circumstances.