

## TOPICAL REVIEW

**First-principles electronic-band calculations on organic conductors**Shoji Ishibashi 2009 *Sci. Technol. Adv. Mater.* **10** 024311 (17pp) doi: [10.1088/1468-6996/10/2/024311](https://doi.org/10.1088/1468-6996/10/2/024311) [Help](#) [PDF \(5.11 MB\)](#) | [References](#)[Shoji Ishibashi](#)

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**Abstract.** Predicting electronic-band structures is a key issue in understanding the properties of materials or in materials design. In this review article, application examples of first-principles calculations, which are not based on adjustable empirical parameters, to study electronic structures of organic conductors are described.

*Keywords:* first-principles calculation, electronic structure, organic conductor

Print publication: Issue 2 (April 2009)

Received 21 December 2008, accepted for publication 2 March 2009

Published 6 July 2009

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