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Band structure diagram paths based on crystallography YOYO HINUMA, Kyoto University, GIOVANNI PIZZI, Ecole Polytechnique Federale de Lausanne, YU KUMAGAI, FUMIYASU OBA, Tokyo Institute of Technology, ISAO TANAKA, Kyoto University — Systematic and automatic calculations of the electronic band structure are a crucial component of computationally-driven high-throughput materials screening. For this purpose, we have derived an algorithm, for any crystal, to derive a unique description of the crystal structure together with a recommended band path [Hinuma *et al.*, http://arxiv.org/abs/1602.06402, Comp. Mater. Sci., accepted.]. The symmetry of the crystal and restrictions on the electronic band structure at Brillouin zone boundaries, which are independent characteristics, are considered and points in reciprocal space are labeled such that there is no conflict with the crystallographic convention. Most notably, we find that a band path that contains all representatives of special k-vector points must depend on the point group in simple and face-centered cubic as well as hexagonal cells. Furthermore, we provide an open-source implementation of the algorithms within our SeeK-path python code, to allow researchers to obtain k-vector coefficients and recommended band paths in an automated fashion. A free online service to compute and visualize the Brillouin zone, labeled k-points and suggested band paths for any crystal structure is available at http://www.materialscloud.org/tools/seekpath/.

Yoyo Hinuma
Kyoto University

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