



## Article

Electronic Structure and Transport Properties of  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  Single Crystals

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**Abstract:** The electrical resistivity and the Hall effect of topological insulator  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  single crystals were studied in the temperature range from 4.2 to 300 K and in magnetic fields up to 10 T. Theoretical calculations of the electronic structure of these compounds were carried out in density functional approach, taking into account spin–orbit coupling and crystal structure data for temperatures of 5, 50 and 300 K. A clear correlation was found between the density of electronic states at the Fermi level and the current carrier concentration. In the case of  $\text{Bi}_2\text{Te}_3$ , the density of states at the Fermi level and the current carrier concentration increase with increasing temperature, from 0.296 states  $\text{eV}^{-1} \text{cell}^{-1}$  (5 K) to 0.307 states  $\text{eV}^{-1} \text{cell}^{-1}$  (300 K) and from  $0.9 \times 10^{19} \text{cm}^{-3}$  (5 K) to  $2.6 \times 10^{19} \text{cm}^{-3}$  (300 K), respectively. On the contrary, in the case of  $\text{Bi}_2\text{Se}_3$ , the density of states decreases with increasing temperature, from 0.201 states  $\text{eV}^{-1} \text{cell}^{-1}$  (5 K) to 0.198 states  $\text{eV}^{-1} \text{cell}^{-1}$  (300 K), and, as a consequence, the charge carrier concentration also decreases from  $2.94 \times 10^{19} \text{cm}^{-3}$  (5 K) to  $2.81 \times 10^{19} \text{cm}^{-3}$  (300 K).

**Keywords:** 2D materials; topological insulator;  $\text{Bi}_2\text{Te}_3$ ;  $\text{Bi}_2\text{Se}_3$ ; electronic structure; DFT; materials informatics; topological resistivity; Hall effect; current carrier concentration



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## 1. Introduction

The quantum Hall effect, in which the Hall conductivity of a two-dimensional insulator in a high magnetic field is quantized, is one of the important discoveries in condensed matter physics [1]. Special conducting edge states appear in the material in the quantum Hall effect regime. This effect is shown to have a topological nature, and such edge states can be associated with a topological invariant called the Chern number [2,3]. A nonzero Chern number determines the presence of conducting edge states, and a zero Chern number means an insulating state in the bulk, which is observed in the quantum Hall effect. Thus, topological materials can be considered as a special state of matter at the intersection of real materials and abstract mathematical topology. Such materials include topological insulators and topological semimetals. The quantum Hall effect can be considered the first two-dimensional topological insulator. Then, three-dimensional topological insulators were theoretically predicted [4,5] and experimentally discovered [6,7]. Recently, Dirac and Weyl topological semimetals were discovered [8–12].

A topological insulator is an insulator or semiconductor in bulk, whereas a special quantum state of electrons occurs on its surface, which makes charge carriers “topologically protected” from scattering. Such surface states are analogues of the edge states in the quantum Hall effect, and the spin–orbit coupling plays a role of the magnetic field. The metallic surface states of a topological insulator are called Dirac cones, which can be

# Electronic Structure And Transport Properties Of Crystals

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