SKiES: The program Implementation of Allen's method for solving kinetic equation for solids from first principles

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The study of transport properties in metals is essential for both the physics of extreme states of matter and fundamental problems in solid-state physics. The most popular theoretical techniques for analyzing the transport characteristics of conductors are those that rely on the solution of the Boltzmann kinetic equation. Allen proposed a strategy [1] for solving the kinetic equation, based on a generalization of the lowest-order variational approximation approach. We introduce our software code, SKiES (Solver of Kinetic Equation for Solids), an implementation of Allen's method. The application facilitates electronic transport calculations from first principles and provides temperature-dependent solid-state transport properties over a broad temperature range. For precise Brillouin zone sampling, the Wannier interpolation approach [2, 3] is employed. The basic functions of the code and the computational workflow are described. Examples of the results for electrical resistivity and thermal conductivity calculations are provided for a range of metals. Convergence issues in the final results are highlighted, particularly those related to the Wannier interpolation procedure.
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[1] Allen P 1978 *Physical Review B* **17** 3725
[2] Marzari N, Mostofi A A, Yates J R, Souza I and Vanderbilt D 2012 *Reviews of Modern Physics* **84** 1419–1475
[3] Giustino F, Cohen M L and Louie S G 2007 *Physical Review B—Condensed Matter and Materials Physics* **76** 165108