Abstract Submitted
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First Principles explanation of the positive Seebeck coefficient of lithium MATTHIEU VERSTRAETE, BIN XU, University of Liege, Belgium — Lithium is one of the simplest metals, with negative charge carriers and a nearly free electron dispersion. Experimentally, however, Li is one of a handful of elements (Cu, Ag, Au) where the sign of the Seebeck coefficient (S) is not that of the carrier. We calculate S fully from first-principles, within P.B. Allen's formulation of Boltzmann theory. The constant relaxation time approximation fails and gives a sign for S necessarily identical to the carriers. Our calculated S are in excellent agreement with experimental data. In comparison with Na, we demonstrate that, within the simplest non-trivial model for the energy dependency of the electron lifetimes, the rapidly increasing density of states (DOS) is related to the sign of S. The exceptional energy dependence of the DOS is beyond the free-electron model, and distorted by the Brillouin Zone edge, a stronger effect in Li than other Alikis. The electron lifetime dependency on energy is central, but details of the electron-phonon interaction are less important, contrary to what has been believed for several decades. The mechanism exposed here may open the door to new "ambipolar" thermoelectric materials, with a tunable sign for the thermopower even if either n- or p-type doping is impossible.

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