

Thermoelectrics Properties Of Weyl Semimetals NbAs

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Faculté : Faculté des Sciences appliquées

Diplôme : Master en ingénieur civil physicien, à finalité approfondie

Année académique : 2025-2026

URI/URL : <http://hdl.handle.net/2268.2/26164>

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Thermoelectric Properties of the Weyl Semimetal NbAs

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Academic year: 2025–2026

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This thesis investigates the thermoelectric properties of the Weyl semimetal NbAs. First-principles calculations based on density functional theory (DFT) were performed to determine its electronic band structure, which served as the foundation for transport modeling. Density functional perturbation theory (DFPT) was subsequently employed to characterize electron–phonon interactions and evaluate the associated scattering processes. The complete set of thermoelectric transport coefficients was then obtained by solving the Boltzmann transport equation, notably through the iterative Boltzmann transport equation (IBTE) approach, allowing the influence of electron doping on transport properties to be assessed.

The results reveal the decisive role of the complex electronic structure and electron–phonon coupling in governing thermoelectric performance. In NbAs, the coexistence of electron and hole pockets at the Fermi level gives rise to a strong bipolar effect. The resulting carrier compensation drastically suppresses the longitudinal Seebeck coefficient, while the high electronic thermal conductivity further limits the thermoelectric figure of merit. Consequently, the maximum figure of merit reaches only $ZT = 0.07$, demonstrating the intrinsic inefficiency of pristine NbAs for thermoelectric energy-conversion applications.

To overcome these limitations, electron-doping strategies were investigated through explicit doping calculations performed within ABINIT and through simulations based on the rigid-band approximation (RBA) using BoltzTraP2. While the RBA predicts a nearly isotropic thermoelectric response, explicit first-principles calculations reveal a strong breakdown of this approximation. Electron doping shifts the Fermi level away from the Weyl nodes and induces a pronounced anisotropy in the Seebeck tensor, leading to strong multiband competition between electron and hole contributions. As a result, conventional chemical doping fails to significantly enhance the thermoelectric efficiency of NbAs.

Representative Work Illustration

The figures below summarize the main results obtained from first-principles DFT, DFPT, and Boltzmann transport calculations.

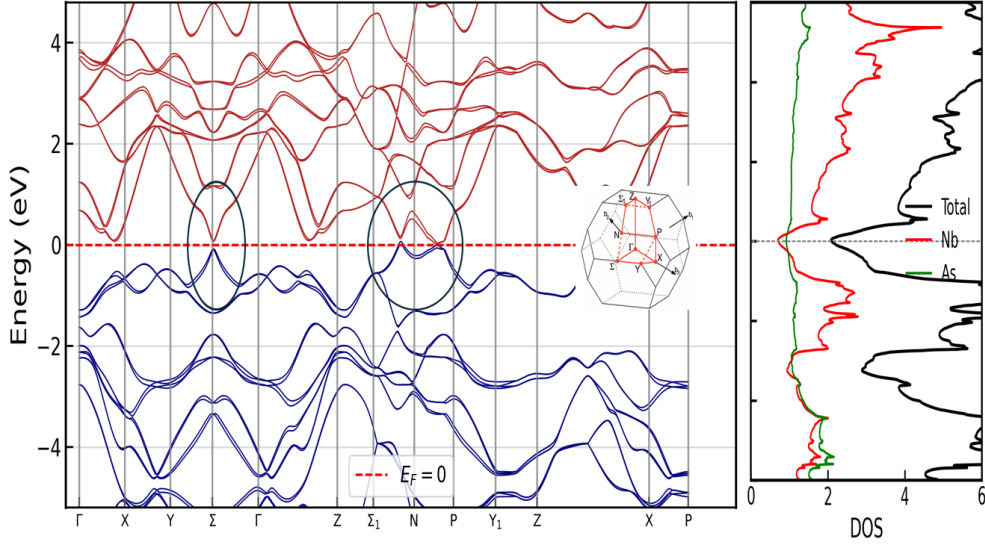


Figure 1: Electronic band structure of NbAs computed on the $16 \times 16 \times 16$ kmesh along the high symmetry path obtained with GGA+ SOC. Together with the density of state (DOS) of NbAs

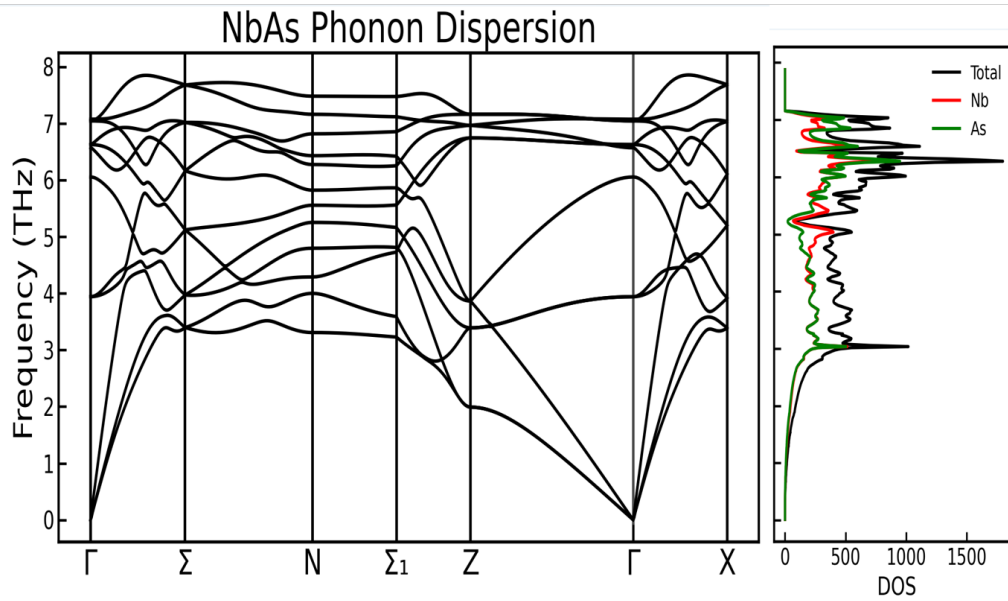
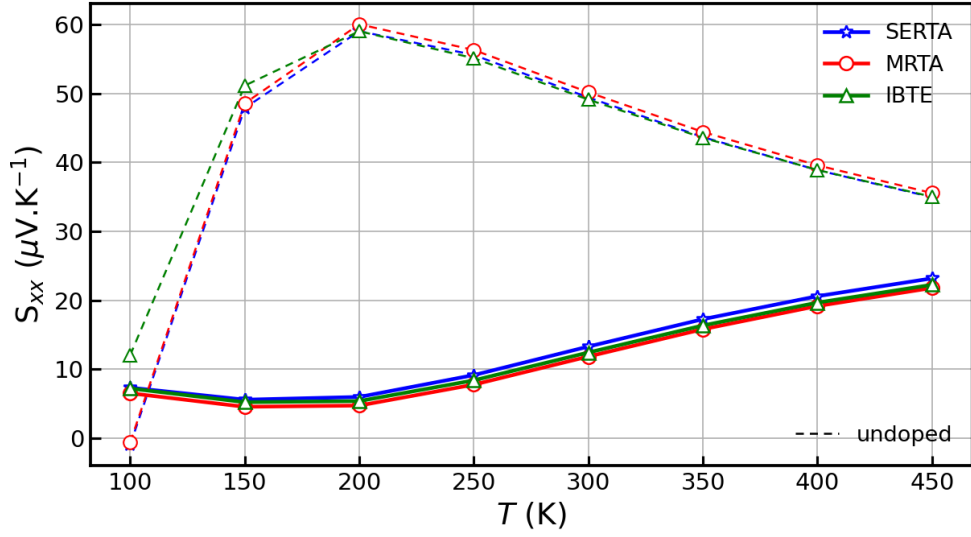
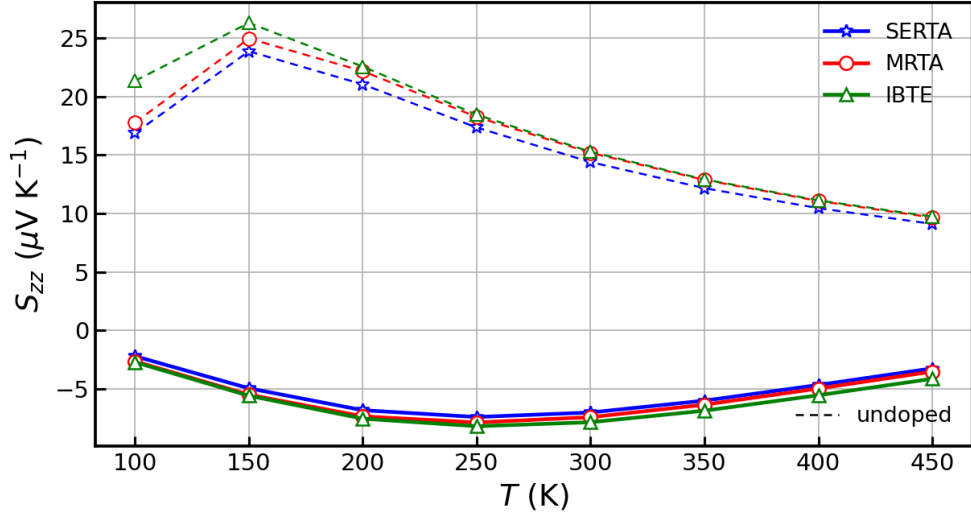


Figure 2: phonon dispersion and phonon density of states of NbAs computed using DFPT on a $4 \times 4 \times 4$ q-point grid along the high symmetry path.

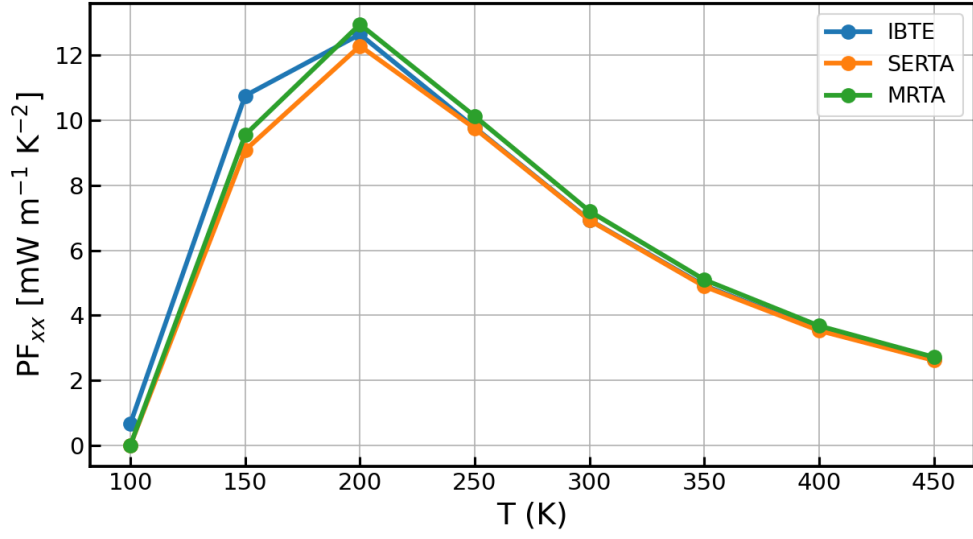


(a)

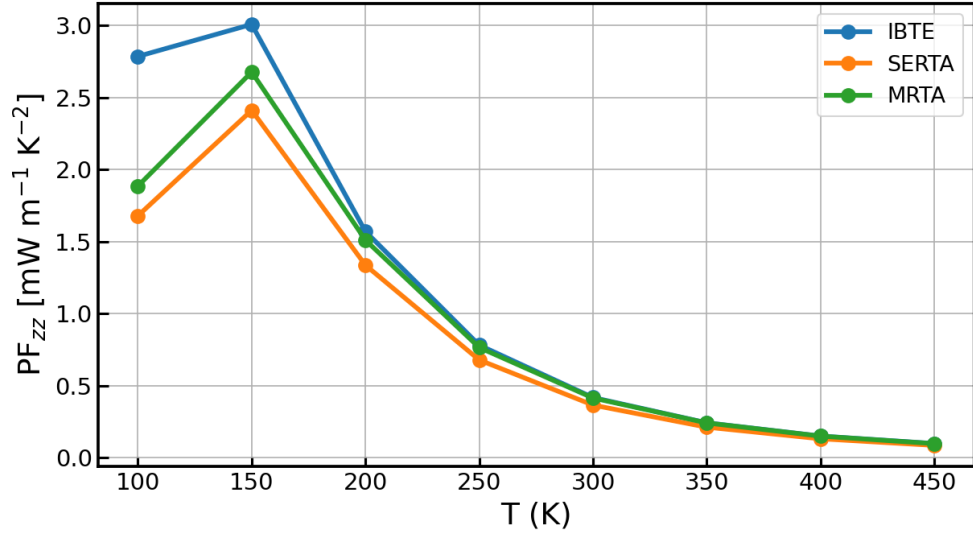


(b)

Figure 3: Temperature dependence of the Seebeck coefficient for heavy n -type doped NbAs ($n = 5 \times 10^{21} \text{ cm}^{-3}$): (a) component S_{xx} and (b) component S_{zz} . The dashed curves display the corresponding intrinsic cases.



(a)



(b)

Figure 4: Temperature dependence of the power factor of NbAs computed using different transport approximations (MRTA, SERTA, IBTE). (a) In-plane PF_{xx} . (b) Out-of-plane PF_{zz}