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DFT prediction of metallic conductivity and experimental investigation of air-induced degradation effects in quasi-one-dimensional antiferromagnet $RbFeSe_2$

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Abstract

A comprehensive study, combining density functional theory (DFT) calculations and experimental investigations, of the quasi-one-dimensional antiferromagnet $RbFeSe_2$ is carried out. The non-spin-polarized ab initio calculations show that its metallic conductivity is above the Néel temperature $T_N = 248$ K, with no gap in the electron density of states at the Fermi energy. The experimental four-probe conductivity measurements yet reveal an insulating behavior throughout the temperature range of 4–300 K. Following these measurements, an X-ray diffraction analysis is conducted. Its results demonstrate a severe degradation of the sample after air exposure (7–9 min), with the reduction in selenium occupancy by more than 20 % below stoichiometric values and the formation of elemental selenium phase ($P3_221$ space group). The discrepancy between theoretical predictions and the obtained experimental results is attributed to the rapid air-induced oxidation leading to structural defects and electron localization. The results obtained highlight the critical importance of rigorous atmospheric control when studying iron chalcogenides, provide quantitative insights into the degradation mechanisms affecting electronic properties, and indicate that standard DFT approaches may overestimate metallicity in quasi-one-dimensional systems, particularly when structural defects are present.

Keywords: *ab initio* calculations, quasi-one-dimensional compound, air-induced degradation, electron localization, iron chalcogenide stability

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ОРИГИНАЛЬНАЯ СТАТЬЯ

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Предсказание металлической проводимости квазиодномерного антиферромагнетика $RbFeSe_2$ в рамках теории функционала плотности и экспериментальное исследование его свойств при деградации на воздухе

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Аннотация

В работе представлены результаты комплексного изучения квазиодномерного антиферромагнетика $RbFeSe_2$ на основе предсказаний в рамках теории функционала плотности (DFT) и экспериментальных данных. Проведенные не спин-поляризованные *ab initio* расчеты предсказывают наличие металлической проводимости выше температуры Неля $T_N = 248$ K и провала в электронной плотности состояний на уровне Ферми. В противоположность этому, методом

четырехконтактного измерения электропроводности установлено изолирующее поведение образца в исследуемом температурном интервале от 4 до 300 K. Анализ рентгеновской дифракции после измерений выявил существенную деградацию свойств образца после воздействия воздуха (7–9 мин): доля селена снизилась более чем на 20 % относительно стехиометрии с образованием элементарного селена (пространственная группа $P3_221$). Обнаруженное несоответствие между теорией и экспериментом объясняется быстрой окислительной деградацией на воздухе, приводящей к структурным дефектам и локализации электронов. Полученные результаты подчеркивают особую важность строгого контроля газовой среды при изучении железосодержащих халькогенидов. Даны количественные оценки механизмов деградации, влияющих на их электронные свойства. Показано, что использование стандартных DFT-подходов может привести к переоценке металлических свойств квазиодномерных систем, особенно при наличии структурных дефектов.

Ключевые слова: *ab initio* расчеты, квазиодномерное соединение, деградация под действием воздуха, локализация электронов, стабильность железосодержащих халькогенидов

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Introduction

Since the discovery of superconductivity in iron-based compounds [1], iron chalcogenides with low-dimensional structures have attracted considerable interest due to their unique electrical and magnetic properties (see numerous reviews [2–10, 14] and references therein). The reduction in dimensionality introduces novel phenomena that do not normally occur in bulk counterparts, such as enhanced quantum fluctuations, geometric frustration, and spin–charge separation [3, 10–14]. These phenomena are associated with the development of exotic magnetic states, unconventional phase transitions, and emergent behavior, offering new avenues for scientific exploration and potential technological applications in quantum computing and spintronics [15, 16].

Iron chalcogenides represent a particularly fascinating subclass within the broader family of iron-based superconductors, distinguished by remarkable structural diversity and electronic properties [2, 17]. Unlike iron pnictides, they exhibit a rich phase diagram encompassing superconducting, magnetic, and insulating phases, often in close proximity to each other [18,19]. The electronic structure of these materials is characterized by strong electron correlations and orbital-dependent interactions, leading to orbital ordering, nematic phases, and unconventional superconducting gap structures [20, 21].

Within iron chalcogenides, there is a subgroup of quasi-one-dimensional compounds with chains of edge-sharing $[FeX_4]$ tetrahedra (X = S, Se, Te), which can be considered as an extreme case of dimensional reduction that amplifies quantum many-body effects [22]. In such systems, the mutual impact of magnetic interactions, structural distortions, and electronic correlations on one another becomes especially pronounced, often yielding complex phase diagrams with multiple competing ground states. The reduced dimensionality can result in spin-Peierls transitions, charge density waves, and metal–insulator transitions driven by magnetic ordering [23, 24].

However, one of the critical challenges in studying iron chalcogenides is their inherent instability in ambient atmospheric conditions. The sensitivity to oxidation can dramatically alter their intrinsic electronic and magnetic properties, leading to discrepancies between theoretical predictions and experimental observations [25, 26]. The most highly air-sensitive compounds are selenides having relatively weak Se–Fe bonds that make them susceptible to oxygen substitution and selenium volatilization. Understanding the above mechanisms is crucial for both fundamental research and potential applications of these materials.

The oxidation processes in iron chalcogenides involve complex chemical reactions that can proceed through multiple pathways, ranging from direct oxygen substitution to formation of oxide phases and elemental chalcogen segregation [27]. They tend to happen very quickly, within minutes of air exposure, and significantly alter the material's electronic structure and transport properties. The defects from oxidation can act as scattering centers, promoting electron localization and suppressing metallic conductivity, even in materials that are theoretically predicted to be metallic.

In the present study, we focus on $RbFeSe_2$, which crystallizes in a monoclinic structure with the $C2/c$ space group [28]. The crystal structure consists of chains of $[FeSe_4]$ tetrahedra sharing common edges and aligned along the crystallographic c-axis. These chains are cross-linked by Rb atoms to form a three-dimensional structure [28]. The quasi-one-dimensional nature of the electronic structure, with preferential electron hopping along the iron chains, makes this compound an ideal candidate for investigating the interplay among dimensionality, magnetic ordering, and electronic transport properties. The magnetic behavior of $RbFeSe_2$ is determined by antiferromagnetic interactions within and between the iron chains. Below the N'eel temperature $T_N = 248$, the antiferromagnetic interactions induce long-range antiferromagnetic ordering [29]. The magnetic structure consists of ferromagnetic chains coupled antiferromagnetically, which together organize into a complex three-dimensional magnetic configuration. This magnetic ordering is expected to have profound effects on the electronic structure, potentially driving a metal–insulator transition as predicted by theoretical models for quasi-one-dimensional magnetic systems.

Previous studies on $RbFeSe_2$ single crystals have utilized measurements of X-ray diffraction, magnetic susceptibility, magnetization, specific heat, as well as Mössbauer spectroscopy [29]. They have conclusively established the basic structural and magnetic properties but so far have failed to address the question of electronic transport and its relationship to the theoretical electronic structure. The absence of systematic conductivity measurements is a critical gap in our understanding of this material, primarily due to the strong predictions for metallic behavior based on available electronic structure calculations.

The theoretical prediction of metallic conductivity in $RbFeSe_2$ above T_N is based on the quasi-one-dimensional electronic structure and the relatively short Fe–Fe distances within the chains. However, the realization of such metallic behavior in practice depends on the structural

integrity of the material and the absence of defects that could lead to electron localization. The Anderson localization mechanism, which is relevant in low-dimensional systems, predicts that even small concentrations of disorder can completely suppress metallic conductivity.

The primary objectives of this work are: (i) to examine the electronic band structure of $RbFeSe_2$ using density functional theory calculations, providing theoretical predictions for the temperature-dependent electronic properties; (ii) to investigate electrical conductivity through direct experimental measurements using four-probe techniques in order to test these theoretical predictions; (iii) to quantitatively analyze the air-induced degradation effects through detailed structural characterization; and (iv) to establish the influence of structural degradation on the observed discrepancies between theoretical predictions and experimental observations. Our approach combines state-of-the-art *ab initio* calculations with careful experimental characterization, including post-measurement structural analysis to assess sample integrity. This comprehensive methodology is helpful in disentangling intrinsic electronic properties from extrinsic effects related to environmental degradation. Our findings reveal the critical importance of atmospheric control in chalcogenide research and provide methodological insights for future investigations of similar environmentally sensitive materials. The broader implications of this work extend beyond the specific compound studied, addressing fundamental questions about the stability and characterization of air-sensitive quantum materials. The quantitative analysis of degradation kinetics and mechanisms provides valuable insights for the design of protective strategies and measurement protocols for similar materials. Furthermore, our results highlight important limitations of existing theoretical approaches when applied to real materials with structural imperfections, contributing to the ongoing dialogue about the predictive power of computational materials science.

1. Theoretical Approach and Experimental Methods

1.1. *Ab initio* calculations. The *ab initio* calculations were based on density functional theory (DFT) [30]. Exchange and correlation effects were treated using the generalized gradient approximation (GGA) as parameterized by the Perdew, Burke, and Ernzerhof (*PBE-sol*) functional [31]. The Kohn–Sham equations were solved using projector-augmented wave (PAW) potentials [32] as implemented in the Vienna *Ab-Initio* Simulation Package (VASP) [33], which is part of the MedeA software suite [34].

Computational parameters were set as follows: plane-wave cutoff of 500 eV, energy tolerance for self-consistency of 10^{-6} eV, and Brillouin zone sampling on Monkhorst–Pack grids of $6\times6\times7$ k-points. Full structure optimization was performed, involving atomic positions, cell dimensions, and shape.

Two magnetic configurations were considered: (i) non-spin-polarized calculations to model the paramagnetic state above the Néel temperature $T_N = 248$ K and (ii) spin-polarized calculations incorporating the antiferromagnetic ground state below T_N. The antiferromagnetic spin configuration was constructed according to neutron diffraction data [28]. This approach enables correct description of temperature-dependent magnetic states during electronic property calculations [35].

It should be noted that standard DFT calculations may have limitations when applied to quasi-one-dimensional systems, particularly regarding the accurate description of correlation effects and potential overestimation of metallic character. These limitations are important to consider when comparing theoretical predictions with experimental results.

1.2. Experimental methods. Single-crystal $RbFeSe_2$ samples were prepared for subsequent electrical conductivity measurements using the four-probe method in a Physical Property Measurement System PPMS-9 (Quantum Design, USA). All measurements were conducted both parallel and perpendicular to the iron chains over the temperature range of 4–300 K.

Sample preparation was performed in a glove box under argon atmosphere to minimize oxidation. However, due to experimental constraints, the samples were exposed to ambient atmosphere for approximately 7–9 min during the transfer from the sealed ampule to the measurement setup. Conductivity measurements were carried out in helium atmosphere.

To investigate potential sample degradation, powder X-ray diffraction studies were performed both on fresh samples and after conductivity measurements. During X-ray diffraction measurements, the samples were coated with an oil-based cryoprotectant (Paratone) to prevent further deterioration.

2. Results and Discussion

2.1. Electronic structure calculations. Fig. 1 shows the calculated electronic band structure and density of states for $RbFeSe_2$ in the paramagnetic regime (temperatures above $T_N = 248$ K). The electron density of states at the Fermi level is significantly non-zero, suggesting that the material exhibits metallic conductivity. The substantial contribution to the density of states around the Fermi level originates from electronic states localized on Fe atoms. Given that the Fe–Fe distance of 2.850(1) Å is only approximately 14 % longer than in metallic iron (2.48 Å) [29], metallic conductivity along the quasi-one-dimensional iron chains would be expected, indicating anisotropic conducting behavior.

The electronic band structure and density of states in the antiferromagnetic regime (below $T_N = 248$ K) are displayed in Fig. 2. A significant band gap separates the valence and conduction bands, pointing to insulating behavior. A comparison between the high- and low-temperature regimes revealed a metal–insulator transition accompanying the magnetic phase transition.

This transition can be understood within the framework of the Hubbard model [36], which predicts that the metal–insulator transition in quasi-one-dimensional systems can be a first-order transition from an antiferromagnetic insulator to a paramagnetic metal. Such transitions have been theoretically established for linear chain lattices, particularly relevant to the $[FeSe_4]$ chain structure in $RbFeSe_2$.

2.2. Experimental conductivity measurements. Contrary to theoretical predictions, the experimental four-probe conductivity measurements revealed no metallic behavior in $RbFeSe_2$ throughout the entire temperature range of 4–300 K, regardless of measurement geometry (parallel or perpendicular to the iron chains). The sample exhibited insulating behavior at all temperatures investigated.

While the insulating behavior below T_N is consistent with the antiferromagnetic DFT calculations, the absence of metallic conductivity above T_N represents a significant discrepancy with theoretical predictions. This discrepancy suggests that factors not accounted for in the idealized DFT calculations may be controlling the experimental transport properties.

2.3. Sample degradation analysis. To understand the origin of the theory–experiment discrepancy, we conducted a detailed structural analysis of the samples after air exposure and measured their conductivity. The powder X-ray diffraction pattern of $RbFeSe_2$ after 7–9 min of air exposure is given in Fig. 3.

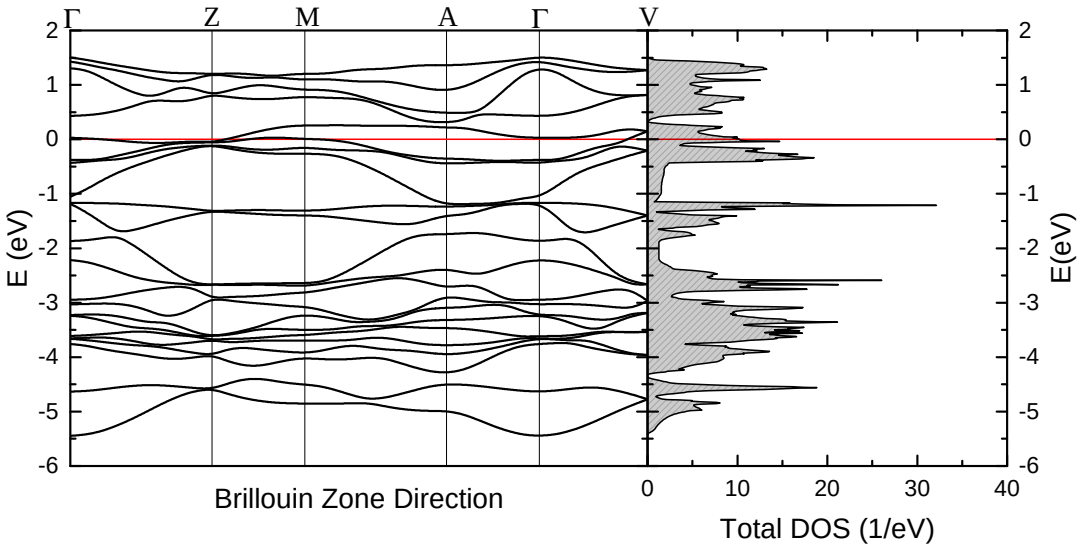

Fig. 1. Calculated band structure and density of states of $RbFeSe_2$ in the non-magnetic state. Notation for the Brillouin zone points is the same as in Ref. [35]. The red horizontal line indicates the Fermi-level energy

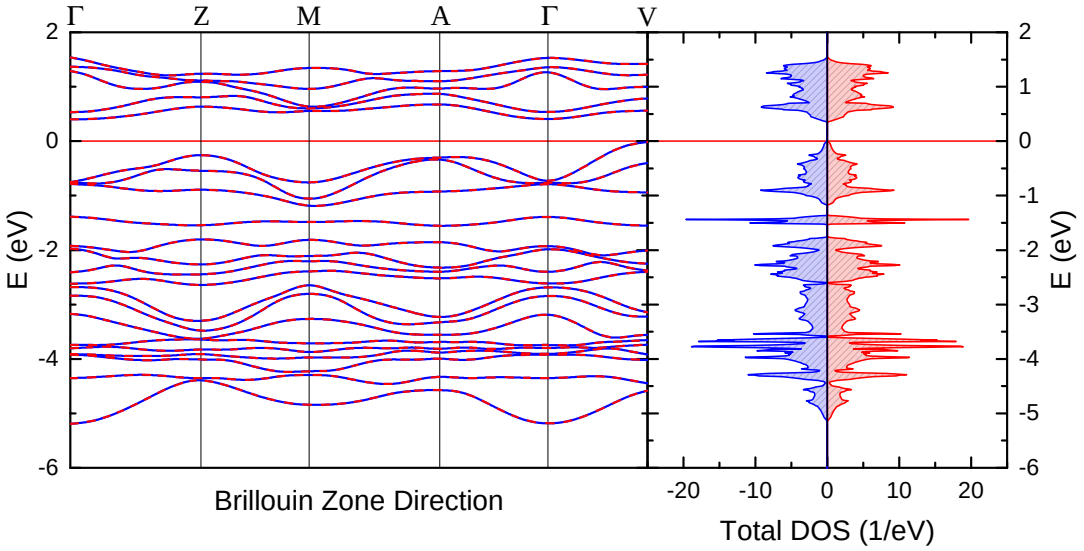

Fig. 2. Calculated band structure and density of states of $RbFeSe_2$ in the antiferromagnetic state. Notation for the Brillouin zone points is the same as in Ref. [35]. The spin-up and spin-down densities and bands are marked with blue and red, respectively

The obtained diffraction pattern reveals a two-phase system: (i) the original $RbFeSe_2$ structure with significantly altered stoichiometry, and (ii) a selenium phase with the $P3_221$ space group symmetry. Critically, the Rietveld refinement demonstrates that the selenium occupancy in the $RbFeSe_2$ phase is reduced by more than 20 % compared to the ideal stoichiometric composition.

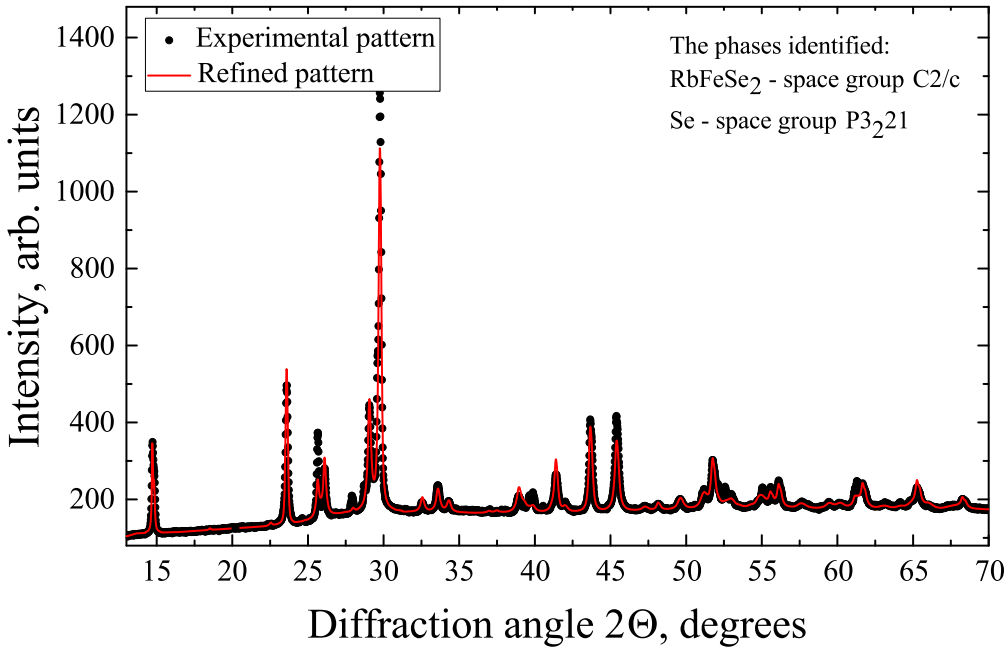

Fig. 3. Powder X-ray diffraction pattern of $RbFeSe_2$ after exposure to ambient atmosphere. The black circles show the measured intensities, and the red solid line corresponds to the refined pattern

This dramatic selenium deficiency can be associated with the following two mechanisms: (i) the formation of selenium vacancies, and (ii) the replacement of selenium with oxygen atoms during air oxidation. The absence of detectable iron oxide phases in the diffraction pattern supports the selenium-to-oxygen substitution mechanism. Such oxidation fundamentally alters the crystal field environment of iron atoms and disrupts the electronic structure of the conducting chains.

2.4. Implications for electronic transport. The observed structural air-induced degradation provides a compelling explanation for the discrepancy between theoretical predictions and experimental observations. In quasi-one-dimensional systems, even relatively small concentrations of defects can lead to electron localization through the Anderson localization mechanisms. The reduction of selenium occupancy factor by more than 20 % represents a substantial defect concentration that would be expected to completely suppress metallic conductivity.

The rapid degradation kinetics (with significant structural changes observed within 7–9 min of air exposure) highlight the extreme sensitivity of $RbFeSe_2$ to oxidative environments. This finding has important implications for both fundamental research and potential applications of iron chalcogenides.

A similar behavior has been reported for the related compound $KFeS_2$ [37,38] when different sample treatment procedures resulted in dramatically different transport properties, ranging from insulating behavior to features of metal–insulator transitions near the Néel temperature. This further supports our conclusion that environmental factors critically influence the observed electronic properties.

2.5. Limitations of DFT approach. Our results also highlight important limitations of standard DFT calculations when applied to quasi-one-dimensional systems. While DFT correctly predicts the electronic structure of ideal, defect-free $RbFeSe_2$, it fails to account for the effects of structural defects that dominate real experimental samples. Additionally, correlation effects, which may be particularly important in quasi-one-dimensional systems, are not fully captured by standard GGA functionals.

Future theoretical investigations should consider: (i) explicit modeling of defect structures and their effects on electronic properties, (ii) including correlation effects through DFT+U or hybrid functional approaches, and (iii) incorporating electron–phonon coupling effects that may influence transport properties.

3. Conclusions

A comprehensive investigation of the electronic properties of quasi-one-dimensional antiferromagnet $RbFeSe_2$ was carried out using a combination of theoretical and experimental approaches. Key findings include:

- **Theoretical predictions:** DFT calculations predict a first-order metal–insulator transition at the Néel temperature ($T_N = 248$ K), with metallic conductivity expected above T_N and insulating behavior below it.
- **Experimental observations:** Four-probe conductivity measurements reveal insulating behavior across the entire temperature range (4–300 K), contradicting theoretical predictions for the paramagnetic regime.
- **Degradation mechanism:** Post-measurement structural analysis indicates that even brief air exposure (7–9 min) induces significant sample degradation, with selenium occupancy reduced by $>20\,\%$ and elemental selenium phase formation.
- **Methodological insights:** The rapid degradation kinetics demonstrate the critical importance of rigorous atmospheric control when studying iron chalcogenides. Standard sample handling procedures may be insufficient to preserve intrinsic electronic properties.
- **Theoretical limitations:** The limitations of standard DFT approaches for quasi-one-dimensional systems, particularly the need to consider correlation effects and defect-induced localization, are shown.

Our work establishes a foundation for understanding degradation mechanisms in quasi-one-dimensional iron chalcogenides and provides methodological guidelines for reliable characterization of these environmentally sensitive materials.

Conflicts of Interest. The authors declare no conflicts of interest.

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