Chapter 5
Rhenium and Tantalum-Based Transition Metal Chalcogenides: Next-Generation Materials for Optoelectronics

Sudipta Koley
https://orcid.org/0000-0002-9174-4229
Department of Physics, Amity Institute of Applied Sciences, Amity University, Kolkata, India

ABSTRACT

Transition metal Dichalcogenides, have emerged as a novel class of two-dimensional layered materials with exceptional potential for optoelectronic applications. Due to their unique electronic band structures, strong light-matter interactions, and tunability, they bridge the gap between conventional semiconductors and low-dimensional nanomaterials. From first-principles density functional theory, the electronic band structure, and optical absorption spectra, of these chalcogenides in mono and few-layer configurations will be studied. Theoretical simulations reveal strong in-plane anisotropic dielectric functions showing their relevance in advanced light detection systems. Tantalum-based dichalcogenides, showcase a rich polymorphic phase encompassing 1T, 1T', and 2H phase. This chapter aims to provide a comprehensive theoretical foundation for researchers exploring novel transition metal dichalcogenide systems for optoelectronics and to highlight the potential of Re- and Ta-based dichalcogenides as advanced functional materials for future electronic and photonic applications.

DOI: 10.4018/979-8-3373-3962-7.ch005

INTRODUCTION

The discovery of stable two-dimensional (2D) materials has introduced a new direction of research in condensed matter physics and materials science owing to their exceptional physical properties and vast potential for integration into next-generation electronic, optoelectronic, and energy devices. The isolation of graphene in 2004 has marked a turning point in research of materials science, stimulating intense research in 2D and van der Waals (vdW) layered systems (Kannan K. et & Tari V. 2025). These atomically thin crystals exhibit quantum confinement effects and surface dominated properties due to reduced dimension, enabling precise control over charge, spin, and light-matter properties at the nanoscale, (Novoselov et al., 2004; Geim & Grigorieva, 2013; Castro Neto et al., 2009). Over the last two decades since this landmark discovery, the field has undergone rapid progress, evolving from exploratory studies of graphene to a diverse and expanding class of 2D chalcogenides. Research on these materials is currently at the forefront of condensed matter physics, physical chemistry, materials science, and nanotechnology, driving interdisciplinary advancements across both fundamental understanding and technological innovation.

For a long time, theoretical arguments based on the Mermin-Wagner theorem suggested that long-range crystalline order in strictly two-dimensional systems like Graphene would be thermodynamically unstable at finite temperatures due to divergent long-wavelength fluctuations (Zakharchenko, 2011.). However, subsequent experimental and theoretical investigations revealed that anharmonic coupling between in-plane and out-of-plane vibrational modes, as well as the stabilizing influence of substrates, give rise to intrinsic out-of-plane vibrations which effectively stabilize 2D crystals (Gurushankar et al., 2024). Thisunderstanding led to a vast range of exploration in monolayer systems. The distinguishing feature of graphene from other conventional materials is its electronic band structure. Its low-energy excitations follow a linear energy-momentum dispersion relation forming massless Dirac fermions in quantum electrodynamics. As a result, electrons and holes in graphene obey a two-dimensional Dirac equation, leading to the emergence of relativistic quantum phenomena in a solid-state context (Katsnelson, 2007). This includes effects such as Klein tunneling, anomalous Landau quantization, and the unconventional half-integer quantum Hall effect which are experimentally confirmed, (Novoselov et al., 2007). The presence of a non-trivial Berry phase of π further confirms the topological nature of charge carriers in graphene, establishing a new paradigm in the field often referred to as relativistic condensed matter physics.

While graphene initially dominated the condensed matter physics research area for a long time, its lack of a bandgap limited its utility in digital electronics and optoelectronic devices. This limitation prompted the search for alternative 2D ma-