Chapter 25
Theoretical Framework of Novel Oxide Compounds for Visible Range Light-Emitting Devices

Sudipta Koley
https://orcid.org/0000-0002-9174-4229
Amity University, Kolkata, India

ABSTRACT

Composite oxides have been proved to be valuable materials in optoelectronic applications. The combination of indium oxide and gallium oxide and other oxides can lead to enhanced optical and electronic properties, making them suitable for a variety of optoelectronic devices. A favorable energy band gap is needed in the visible region of the spectrum, indicating the applicability in optoelectronic devices such as LEDs and solar cells. Overall band gap engineering and tuning the radiative recombination is a challenge for new age semiconductors. Artificial Intelligence and Machine Learning have become powerful tools in the theoretical study and discovery of oxide materials for LEDs. By analyzing vast datasets, models can predict material properties, optimize synthesis parameters, and even generate new compounds with desired characteristics. This data-driven approach accelerates the material discovery process and enhances the precision of theoretical predictions, allowing researchers to explore a broader chemical space and identify optimal candidates for visible range light emission.

1. INTRODUCTION

The quest for efficient, durable, and versatile light-emitting devices (LEDs) has been a central focus of research in material science and optoelectronics [Huang et al.,2020; Liu et al.,2024]. LEDs have revolutionized the fields of display technology, solid-state lighting, and even medical devices, owing to their energy efficiency, long lifespan, and environmental benefits compared to traditional incandescent and fluorescent lighting [Pode,2020; Kwon et al., 2020; Zou et al., 2020]. The foundation of these devices lies in the materials that emit light, traditionally dominated by III-V semiconductor compounds like gallium nitride. However, as the demand for better performance and new functionalities grows, the search for alternative materials that can operate effectively in the visible range has intensified. Among these alter-

DOI: 10.4018/979-8-3693-7974-5.ch025

natives, oxide semiconductors have emerged as promising candidates due to their unique properties and potential for band gap engineering [Chaves et al.,2020; Rodrigues et al.,2024; Kumbhakar et al., 2021].

Oxide semiconductors stand out in the landscape of light-emitting materials for several reasons. Firstly, oxides generally possess excellent thermal and chemical stability, making them robust in various operating conditions, a crucial factor for the longevity and reliability of LEDs. Secondly, many oxides naturally exhibit wide band gaps, which can be finely tuned to produce light in the visible spectrum. This tunability is vital for creating LEDs that can emit specific colors or white light with high color rendering indices. Moreover, oxide materials are abundant and often less expensive to produce than their III-V counterparts. This cost-effectiveness, coupled with their environmental friendliness, positions oxide semiconductors as attractive materials for large-scale, sustainable production of LEDs. The ongoing exploration of novel oxide compounds is driven by the need to discover materials with better performance characteristics like higher efficiency, brighter emission, and greater flexibility in device integration [Ren et al.,2021; Min et al.,2024].

The visible spectrum, ranging from approximately 380 nm (violet) to 750 nm (red), is critical for most LED applications, including general lighting, displays, and indicators. Achieving efficient light emission within this range requires precise control over the band gap of the emitting material. Traditional LED materials like GaN and InGaN have been successfully used to produce blue and green light, but creating efficient and stable red and orange LEDs has been more challenging [Liu et al.,2022; Bean et al., 1985]. Oxide semiconductors offer a pathway to overcome these challenges, as their band structures can be engineered to cover the entire visible spectrum. By tuning the electronic and optical properties of these oxides, LEDs can be developed which emit across the visible range with high efficiency and stability. The discovery and optimization of novel oxide compounds for visible-range LEDs rely heavily on theoretical studies. Computational methods and theoretical models provide the necessary insights into the electronic structure, and optical properties of these materials, allowing researchers to predict their behavior without any experimental results. This predictive power is crucial for identifying promising materials, optimizing their composition and processing conditions, and understanding the fundamental mechanisms that govern their performance.

Theoretical approaches such as density functional theory (DFT), time-dependent DFT, and many-body perturbation theory have become indispensable tools in materials research. All these theoretical tools allow for the exploration of complex phenomena such as electron-phonon interactions, excitonic effects, and the influence of defects and impurities on light emission. Additionally, density functional theory predictions for proposed materials about formation energy and strain effects can guide future experiments.

This chapter is structured to provide a comprehensive theoretical framework for understanding and designing novel oxide compounds for visible-range light-emitting devices. It begins with a discussion of the fundamental principles of light emission in semiconductors, focusing on the mechanisms that allow these materials to emit photons in the visible spectrum. Following this, the chapter explores the unique properties of oxide semiconductors, including their crystal structures, electronic properties, and the role of dopants in shaping their optical behavior. Special emphasis is placed on the concept of band gap engineering, a critical factor in tuning the emission properties of oxides. Theoretical models and computational methods that are used to predict and optimize these properties are discussed later, providing the reader with a clear understanding of the tools available to researchers in this field. The chapter will also explore more advanced topics, such as the interaction of phonons with charge carriers and its impact on non-radiative recombination losses, the design of heterostructures and quantum wells in oxide LEDs, and the use of theoretical modeling to guide the discovery of new materials. By presenting examples