

Electronic Structure, Optical and Transport Properties of Double Perovskite $\text{La}_2\text{NbMnO}_6$: A Theoretical Understanding from DFT Calculations

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Double perovskite $\text{La}_2\text{NbMnO}_6$ was systematically studied using the first-principles calculations. The structural, electronic, optical and transport properties of this compound were calculated. Spin resolved band structure predicted this material as a half-metal with an energy gap of 3.75 eV in spin down state. The optical coefficients including optical conductivity, reflectivity and electron energy loss are calculated for photon energy up to 30.00 eV to understand the optical response of this perovskite. The strong absorption of all the ultraviolet and infrared frequencies of the spectrum by this material may suggest the potential application of this material for the optoelectronic devices in ultraviolet and infra-red region. Also, the thermoelectric properties with a speculation from the half-metallic electronic structure are reported. Subsequently, the Seebeck coefficient, electrical and thermal conductivity coefficients are calculated to predict the thermoelectric figure of merit (zT), the maximum of which is found out to be 0.14 at 800 K.

Key words: Double perovskites, DFT calculations, electronic structure, transport and thermodynamic properties

INTRODUCTION

Perovskites are listed in the multifunctional class of compounds due to their unique electronic structure and wide-ranging electronic, chemical and mechanical properties. Without considerable change in the crystal structure, their composition can be altered by a wide range of dopant atoms (subject to the Goldschmidt tolerance factor), and this flexibility allows the modification of the

attractive physical and chemical properties.^{1,2} Consequently, the alternative or lead-free materials for device application can be designed. A huge potential for many energy conversion processes is bestowed by such compounds due to their insulating, half-metallic, semiconducting, metallic or even superconducting transport properties. Ferromagnetic, multiferroic, piezoelectric, dielectric, catalytic or thermoelectric materials are also known in this family.^{3–5} Global warming and the limited supply of fossil fuels are the major challenges, which can only be met by the development of new energy conversion, renewable resources and storage technologies.

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