SpringerBriefs in Materials

Rachid Masrour

# Magnetoelectronic, Optical, and Thermoelectric Properties of Perovskite Materials

Springer

# SpringerBriefs in Materials

The SpringerBriefs Series in Materials presents highly relevant, concise monographs on a wide range of topics covering fundamental advances and new applications in the field. Areas of interest include topical information on innovative, structural and functional materials and composites as well as fundamental principles, physical properties, materials theory and design.

**Indexed in Scopus (2022)**.

SpringerBriefs present succinct summaries of cutting-edge research and practical applications across a wide spectrum of fields. Featuring compact volumes of 50 to 125 pages, the series covers a range of content from professional to academic. Typical topics might include

- A timely report of state-of-the art analytical techniques
- A bridge between new research results, as published in journal articles, and a contextual literature review
- A snapshot of a hot or emerging topic
- An in-depth case study or clinical example
- A presentation of core concepts that students must understand in order to make independent contributions

Briefs are characterized by fast, global electronic dissemination, standard publishing contracts, standardized manuscript preparation and formatting guidelines, and expedited production schedules.

Rachid Masrour

# Magnetoelectronic, Optical, and Thermoelectric Properties of Perovskite Materials

Springer

Rachid Masrour
Laboratory of Solid Physics
Faculty of Sciences Dhar El Mahraz
Sidi Mohamed Ben Abdellah University
Fez, Morocco

ISSN 2192-1091 ISSN 2192-1105 (electronic)
SpringerBriefs in Materials
ISBN 978-3-031-48966-2 ISBN 978-3-031-48967-9 (eBook)
https://doi.org/10.1007/978-3-031-48967-9



This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Paper in this product is recyclable.

# General Introduction

The perovskite oxide is a versatile class of compounds with A-site being 12 coordinated and occupied by rare earth or alkaline earth ions with large ionic radii. The B-site being octahedrally coordinated and generally occupied by a transition metal ion or rare earth ion with smaller ionic radii. It contains corner sharing $BO_6$ octahedra and the voids are filled by the larger radius A cations. Perovskite solar cells have attracted extensive attention due to their excellent optoelectronic properties, low cost, and easy fabrication, among other qualities [1–3]. Because of lead's high toxicity for the environment and humans, the industrial application of lead-based perovskites has been greatly limited [4, 5]. Currently, perovskite solar cells hold a record efficiency of 25.6% in a laboratory scale [6]. For organic-inorganic hybrid perovskites, secondary growth is usually achieved by a post-synthetic treatment induced in-situ transformation to perovskites with reduced dimension and higher stability, especially along the defect-rich grain boundaries [7]. Inorganic perovskites, exemplified by $CsPbI_3$, are characterized by superior chemical stability compared to their organic A-site cation counterparts. However, they do exhibit a higher density of defects. Nevertheless, achieving an organized secondary arrangement or reconstruction in these inorganic perovskites with reduced defects presents a significant challenge due to their distinctive chemical properties [8]. The performance of perovskite photodetectors has made a breakthrough in a short time. At present, the perovskite photodetectors with external quantum efficiency over 90% have been realized [8], and the external quantum efficiency (EQE) can be further enhanced by introducing photomultiplication (PM) effect. Moreover, some special properties, such as oxygen vacancies and the change in the B-site ion valence state, will significantly influence the catalytic activity of these perovskite materials [9]. Additionally, perovskite oxides can be made into different types of sensors, e.g., current and capacitance sensors, which are based on their various electrochemical properties such as good conductivity and dielectric properties [10, 11]. The research in the area of A-site ordering of this family of double perovskites is less compared to the B-site ordering. The result of these rare studies of A-site ordering is particularly due to the fact that most of the materials with these sorts of ordering needs high pressure synthesis and exist over a very narrow range of temperature [12–14]. Previous studies have shown that

$La_2NiTiO_6$ and $La_2MnTiO_6$ exhibit long-range paramagnetism at room temperature, which can explain laterally that Ti does not exhibit antiferromagnetism macroscopically in the double perovskite system, eliminating the risk of introducing additional antiferromagnetic particles [15, 16]. Previous researchers have found many interesting properties in halide perovskites [17–19], due to their complicated structure and noncentral symmetry, especially when transition metal (TM) ions are incorporated or used [20–22]. Recently, chalcogenide perovskites have received increased attention as an emerging ionic semiconductor family with fascinating optoelectronic properties [23–28]. The electronic, magnetic and magnetocaloric properties of $T_{1-x}Sr_xMnO_3$ with (T=La, Pr) and ($x = 0.35$ and $0.25$) were studied by using the density functional theory and Monte Carlo study with the generalized gradient GGA, GGA+U (Hubbard parameter) and the Modified Becke-Johnson approximation. The Monte Carlo simulations were used to calculate some magnetic parameters such as the exchange coupling constants and magnetic moments. The electronic, optical, thermoelectric, magnetic, and magnetic properties of the $GdCrO_3$ system by using the DFT and Monte Carlo simulation. We have studied the magnetic properties and magnetocaloric effect in $Sr_2FeMoO_6$, $La_2SrMn_2O_7$ bilayer manganite, the surface effects on the magnetocaloric properties of perovskites ferromagnetic thin films, $SmFe_{1-x}Mn_xO_3$ perovskite.

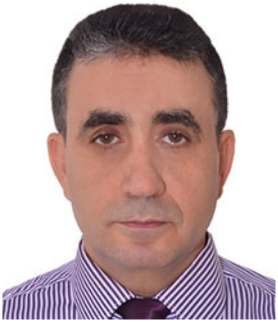
## References


1. A. Farokhi, H. Shahroosvand, G. Delle Monache, M. Pilkington, M.K. Nazeeruddin, The evolution of triphenylamine hole transport materials for efficient perovskite solar cells, Chem. Soc. Rev. 51 (2022) 5974–6064.
2. P. Mahajan, B. Padha, S. Verma, V. Gupta, R. Datt, W.C. Tsoi, S. Satapathi, S. Arya, S, Review of current progress in hole-transporting materials for perovskite solar cells, J. Energy Chem. 68 (2022) 330–386.
3. X.X. Yin, Z.N. Song, Z.F. Li, W.H. Tang, toward ideal hole transport materials: a review on recent progress in dopant-free hole transport materials for fabricating efficient and stable perovskite solar cells, Energy Environ. Sci. 13 (2020) 4057–4086.
4. M. Ren, X. Qian, Y. Chen, T. Wang, Y. Zhao, Potential lead toxicity and leakage issues on lead halide perovskite photovoltaics, J. Hazard Mater. 426 (2022) 127848.
5. A. Babayigit, A. Ethirajan, M. Muller, B. Conings, Toxicity of organometal halide perovskite solar cells, Nat. Mater. 15 (2016) 247–251.
6. J.J. Yoo, G. Seo, M.R. Chua, T.G. Park, Y. Lu, F. Rotermund, Y.-K. Kim, C.S. Moon, N.J. Jeon, J.-P. Correa-Baena, V. Bulovi_c, S.S. Shin, M.G. Bawendi, J. Seo, Efficient perovskite solar cells via improved carrier management, Nature 590 (2021) 587–593, https://doi.org/10.1038/s41586-021-03285-w
7. Grancini G, Nazeeruddin MK. Dimensional tailoring of hybrid perovskites for photovoltaics. Nat Rev Mater 2019; 4:4–22.
8. Yuetian Chen, Xingtao Wang, Yao Wang, Xiaomin Liu, Yanfeng Miao, Yixin Zhao. Functional organic cation induced 3D-to-0D phase transformation and surface reconstruction of CsPbI3 inorganic perovskite. https://doi.org/10.1016/j.scib.2023.03.029
9. J. Miao, F. Zhang, Recent progress on highly sensitive perovskite photodetectors, J. Mater. Chem. C 7 (2019) 1741–1791.

10. Juan He, Xiaomin Xu, Meisheng Li, Shouyong Zhou, Wei Zhou. Recent advances in perovskite oxides for non-enzymatic electrochemical sensors: A review. Analytica Chimica Acta 1251 (2023) 341007
11. F. Malvano, L. Maritato, G. Carapella, P. Orgiani, R. Pilloton, M. Di Matteo, D. Albanese, Fabrication of SrTiO3 layer on Pt electrode for label-free capacitive biosensors, Biosensors 8 (2018) 26, https://doi.org/10.3390/bios8010026
12. U.T. Nakate, P. Patil, Y.T. Nakate, S.I. Na, Y.T. Yu, Y.B. Hahn, Ultrathin ternary metal oxide Bi2MoO6 nanosheets for high performance asymmetric supercapacitor and gas sensor applications, Appl. Surf. Sci. 551 (2021), 149422, https://doi.org/10.1016/j.apsusc.2021.149422
13. Y. Long, T. Saito, T. Tohyama, K. Oka, M. Azuma, Y. Shimakawa Inorganic Chemistry, 48 (2009), p. 8489
14. Y. Long, T. Kawakami, W. Chen, T. Saito, T. Watanuki, Y. Nakakura, Q. Liu, C. Jin, Y. Shimakawa Chem. Mater., 24 (2012), p. 2235
15. A. Aimi, D. Mori, K. Hiraki, T. Takahashi, Y.J. Shan, Y. Shirako, J. Zhou, Y. Inaguma Chem. Mater., 26 (2014), p. 2601
16. U. Dutta, A. Haque, M.M. Seikh, Synthesis, structure and magnetic properties of Ti doped La2MnNiO6 double perovskite, Chimica Techno Acta, 6 (2019) 80–92.
17. D.M.A. Jaimes, J.M. De Paoli, V. Nassif, P.G. Bercoff, G. Tirao, R.E. Carbonio, F. Pomiro, Effect of B-Site order-disorder in the structure and magnetism of the new perovskite family La2MnB'O6 with B' = Ti, Zr, and Hf, Inorg. Chem., 60 (2021) 423 4935–4944.
18. C.B. Samantaray, H. Sim, H. Hwang, Microelectron. J. 36 (2005) 725.
19. H. Muta, K. Kurosaki, S. Yamanaka, J. Alloys Compd. 350 (2003) 292.
20. N.O. Damerdji, B. Amrani, K.D. Khodja, P. Aubert, J. Supercond. Nov. Magnetism 31 (2018) 2935.
21. K. Xu, C. Lin, X. Xie, A. Meijerink, Chem. Mater. 29 (2017) 4265.
22. G. Pan, X. Bai, D. Yang, X. Chen, P. Jing, S. Qu, L. Zhang, D. Zhou, J. Zhu, W. Xu, B. Dong, H. Song, Nano Lett. 17 (2017) 8005.
23. K. Xu, A. Meijerink, Chem. Mater. 30 (2018) 5346.
24. Y.-Y. Sun, M.L. Agiorgousis, P. Zhang, S. Zhang, Chalcogenide Perovskites for Photovoltaics, Nano Lett. 15 (1) (2015) 581–585.
25. S. Perera, H. Hui, C. Zhao, H. Xue, F. Sun, C. Deng, N. Gross, C. Milleville, X. Xu, D. F. Watson, B. Weinstein, Y.-Y. Sun, S. Zhang, H. Zeng, Chalcogenide perovskites - an emerging class of ionic semiconductors, Nano Energy 22 (2016) 129–135.
26. X. Wei, et al., Realization of BaZrS3 chalcogenide perovskite thin films for optoelectronics, Nano Energy 68 (2020), 104317.
27. S. Niu, H. Huyan, Y. Liu, M. Yeung, K. Ye, L. Blankemeier, T. Orvis, D. Sarkar, D. J. Singh, R. Kapadia, J. Ravichandran, Bandgap Control via Structural and Chemical Tuning of Transition Metal Perovskite Chalcogenides, Adv. Mater. 29 (9) (2017) 1604733, https://doi.org/10.1002/adma.v29.910.1002/adma.201604733
28. I. Sadeghi, K. Ye, M. Xu, Y. Li, J.M. LeBeau, R. Jaramillo, Making BaZrS3 Chalcogenide Perovskite Thin Films by Molecular Beam Epitaxy, Adv. Funct. Mater. 31 (45) (2021) 2105563, https://doi.org/10.1002/adfm.v31.4510.1002/adfm.202105563
29. K. Hanzawa, S. Iimura, H. Hiramatsu, H. Hosono, Material design of green-lightemitting semiconductors: Perovskite-type sulfide SrHfS3, J. Am. Chem. Soc. 141 (13) (2019) 5343–5349

# Contents

# About the Author



**Prof. Rachid Masrour** from Morocco, actually, is a research professor in the Faculty of Sciences Dhar El Mahraz at Sidi Mohamed Ben Abdellah the University, Fez, Morocco. Dr. Rachid Masrour completed his Ph.D. in March 2006 at the same University. His research interests lie in the areas of Condensed Matter Physics, Material Sciences, Material for energy, Magnetism, etc.… He has 340 articles published in Web of Science and 10 book chapters published in international journals, editor of 8 Books and author of 2 books with an h-index of 34. He participated in more than 100 Moroccan and international congress. He's a Referee of several articles and also an Editorial Board Member in different international journals. He has a lot of collaboration with laboratories from abroad. He has been honored with the International Association of Advanced Materials Young Scientist Medal in recognition for his contribution to "Magnetism, Electromagnetism and Spintronics" and delivered a lecture at the Advanced Materials World Congress on 11-14 October 2022. One of the world's most cited top scientists in material physics (top 2%, Stanford University Ranking, US, 2020 and in 2023). He has the Best Oral Presentation Award for MCGPD-2021, by Indian Association for Crystal Growth & Indian Science and Technology Association International Organization for Crystal Growth, 5-8, July 2021. Outstanding Scientist Award (VDGOOD PROFESSIONAL ASSOCIATION, 15-02-2020, India). It was among the most critical in 2020 by Elsevier.