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Rachid Masrour



Magnetoelectronic, Optical, and Thermoelectric Properties of Perovskite Materials

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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

$\text{La}_2\text{NiTiO}_6$ and $\text{La}_2\text{MnTiO}_6$ 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 $\text{T}_{1-x}\text{Sr}_x\text{MnO}_3$ with ($\text{T}=\text{La}, \text{Pr}$) 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 $\text{Sr}_2\text{FeMoO}_6$, $\text{La}_2\text{SrMn}_2\text{O}_7$ bilayer manganite, the surface effects on the magnetocaloric properties of perovskites ferromagnetic thin films, $\text{SmFe}_{1-x}\text{Mn}_x\text{O}_3$ 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 CsPbI_3 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. Damerdjii, 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.v29.9.10.1002/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.v31.45.10.1002/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

1	Calculation Methods: Monte Carlo Simulations and Ab Initio Calculations	1
1.1	Introduction	1
1.2	Monte Carlo Method and Ising Model	2
1.3	Ab-Initio Calculations	7
1.4	Several Approximations	8
1.4.1	Born–Oppenheimer Approximation	8
1.4.2	Hartree Approximation	9
1.4.3	Hartree–Fock Approximation	10
1.5	Density Functional Theory	11
1.5.1	Theorems of Hohenberg and Kohn	11
1.5.2	Formulation of Kohn–Sham	12
1.5.3	Local Density of Approximation	13
1.5.4	Generalized Gradient Approximation	14
1.6	Conclusion	15
	References	15
2	Magnetocaloric Effect, Electronic and Magnetic Properties in Manganite Perovskites	17
2.1	Introduction	17
2.2	Calculation Details: Density-Functional Theory and Monte Carlo Simulations	18
2.3	Crystal Structure of Manganite Perovskite	20
2.4	Electronic Properties of Manganite Perovskite	21
2.5	Magnetic and Magnetocaloric Properties of Manganite Perovskite	27
2.6	Conclusions	35
	References	36

3	Study of Magnetocaloric Effect, Electronic and Magnetic Properties of Perovskite Ferrites	39
3.1	Introduction	39
3.2	Density-Functional Theory and Monte Carlo Simulations	40
3.3	Crystal Structure of Ferrite Perovskite	43
3.4	Electronic Properties of Ferrite Perovskite	44
3.5	Magnetic and Magnetocaloric Properties of Ferrite Perovskites	49
3.6	Conclusions	54
	References	56
4	Magnetic and Magnetocaloric, Electronic, Magneto-Optical, and Thermoelectric Properties of Perovskite Chromites	59
4.1	Introduction	59
4.2	Calculation Methods	60
4.2.1	Density Functional Theory	60
4.2.2	Monte Carlo Study	60
4.3	Crystal Structure of Perovskite Chromites	63
4.4	Electronic Properties of Perovskite Chromites	64
4.5	Dielectric and Optical Properties of Perovskite Chromites	65
4.6	Thermoelectric Properties of Perovskite Chromites	69
4.7	Magnetic and Magnetocaloric Effect of Perovskite Chromites	71
4.8	Conclusions	73
	References	74
5	Magnetic Properties and Magnetocaloric in Double Perovskite Oxides	77
5.1	Introduction	77
5.2	Ising Model and Monte Carlo Simulations	78
5.3	Results and Discussion of Magnetic Properties and Magnetocaloric in Double Perovskite Oxides	81
5.4	Conclusions	82
	References	85
6	Magnetocaloric and Magnetic Properties of Bilayer Manganite	87
6.1	Introduction	87
6.2	Ising Model and Monte Carlo Simulations	88
6.3	Magnetic and Magnetocaloric Properties of Bilayer Manganite System	90
6.4	Conclusions	92
	References	93
7	Magnetocaloric Properties of Surface Effects in Perovskites Ferromagnetic Thin Films	95
7.1	Introduction	95
7.2	Ising Model and Monte Carlo Simulations	96
7.3	Results and Discussion: Surface Effects in Perovskites Ferromagnetic Thin Films	99

7.4	Conclusions	107
	References	107
8	Effect of Magnetic Field on the Magnetocaloric and Magnetic Properties of Perovskite Orthoferrites	109
8.1	Introduction	109
8.2	Ising Model and Monte Carlo Study	110
8.3	Results and Discussion: Magnetocaloric Effect and Magnetic Properties of Perovskite Orthoferrites	112
8.4	Conclusions	116
	References	117
	General Conclusion	119

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