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Modeling the structure of a lead-free perovskite solar cell

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The article discusses the numerical simulation of a lead-free perovskite solar cell in the SCAPS-1D program to optimize its structure and improve the energy conversion efficiency.

The influence of the thickness, concentration of defects and acceptors in the layer of lead-free perovskite $CH_3NH_3SnI_3$, as well as the work function of the back contact material on the photovoltaic parameters of a solar cell has been studied. It was found that the optimal thickness of the $CH_3NH_3SnI_3$ layer is 500 nm, the concentration of defects should be on the order of 10^{14}–10^{15} cm^{-3}, and the optimal concentration of acceptors should be 10^{16} cm^{-3}. It is shown that the work function of the rear contact material must be at least 4.9–5 eV to create highly efficient solar cells. A maximum efficiency of 23.13 % was obtained for a perovskite solar cell with the FTO/TiO_2/$CH_3NH_3SnI_3$/Cu_2O/C structure (short circuit current 31.94 mA/cm^2, open circuit voltage 0.95 V, fill factor 76.07 %). The results can be used in the design and manufacture of non-toxic, high-performance and low-cost perovskite solar cells.

Keywords: solar cell, numerical simulation, lead-free perovskite, defect concentration, layer thickness, acceptor concentration, back contact.

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REFERENCES

1. Linfeng Cai and Furong Zhu, Nano Select **2**, 1417 (2021).
2. N. Suresh Kumar and K. Chandra Babu Naidu, Journal of Materiomics **7**, 940 (2021).
3. Weifu Sun, Kwang-Leong Choy, and Mingqing Wang, Molecules **24**, 3466 (2019).
4. M. Mottakin, K. Sobayel, Dilip Sarkar, Hend Alkhammash, Sami Alharthi, Kuaanan Techato, Md. Shahiduzzaman, Nowshad Amin, Kamaruzzaman Sopian, and Md. Akhtaruzzaman, Energies **14**, 7200 (2021).
5. Hui-Jing Du, Wei-Chao Wang, and Jian-Zhuo Zhu, Chin. Phys. B **25**, 108803 (2016).
6. Saquib Ahmed, Jalen Harris, Jon Shaffer, Mohan Devgun, Shaestagir Chowdhury, Aboubakr Abdullah, and Sankha Banerjee, Journal of Materials Research **34**, 2789 (2019).
7. Mingzhen Liu, Michael B. Johnston, and Henry J. Snaith, Nature **501**, 393 (2013).
8. D. A. Kudryashov, A. S. Gudovskikh, A. V. Babichev, A. V. Filimonov, A. M. Mozharov, V. F. Agekyan, E. V. Borisov, A. Yu. Serov, and N. G. Filosofov, Semiconductors **51**, 11 (2017).
9. F. Behrouznejad, S. Shahbazi, N. Taghavinia, Hui-Ping Wud, and Eric Wei-Guang Diau, J. Mater. Chem. A **4**, 13488 (2016).
10. M. Burgelman, P. Nollet, and S. Degrave, Thin Solid Films **361–362**, 527 (2000).
11. T. Minemoto and M. Murata, J. of Appl. Phys. **116**, 054505 (2014).
12. Himanshu Dixit, Deepak Punetha, and Saurabh Kumar Pandey, International Journal for Light and Electron Optics **179**, 969 (2019).
13. S. P. Malyukov, A. V. Sayenko, and A. V. Ivanova, IOP Conf. Series: Materials Science and Engineering **151**, 012033 (2016).
14. A. V. Sayenko, S. P. Malyukov, A. V. Palii, and E. V. Goncharov, Applied Physics, No. 2, 45 (2021).
15. Takashi Minemoto, Yu Kawano, Takahito Nishimura, and Jakapan Chantana, Optical Materials **92**, 60 (2019).
16. S. Abdelaziz, A. Zekry, A. Shaker, and M. Abouelatta, Optical Materials **101**, 109738 (2020).
17. Neelima Singh, Alpana Agarwal, and Mohit Agarwal, Solar Energy **208**, 399 (2020).
18. Yu Kawano, Jakapan Chantana, Takahito Nishimura, and Takashi Minemoto, Solar Energy Materials and Solar Cells **205**, 110252 (2020).
19. Huanping Zhou, Qi Chen, Gang Li, Song Luo, Tze-bing Song, Hsin-Sheng Duan, Ziruo Hong, Jingbi You, Yongsheng Liu, and Yang Yang, Science **345**, 542 (2014).
20. Tejas S. Sherkar, Cristina Momblona, Lidon Gil-Escrig, Jorge Avila, Michele Sessolo, Henk J. Bolink, and L. Jan Anton Koster, ACS Energy Letters **2**, 1214 (2017).
21. Feng Hao, Constantinos C. Stoumpos, Peijun Guo, Nanjia Zhou, Tobin J. Marks, Robert P. H. Chang, and Mercouri G. Kanatzidis, J. Am. Chem. Soc. **137**, 11445 (2015).
22. Feng Hao, Constantinos C. Stoumpos, Duyen Hanh Cao, Robert P. H. Chang, and Mercouri G. Kanatzidis, Nature Photonics **137**, 489 (2015).