

SYNTHESIS AND ANALYSIS OF AROMATIC ORGANIC ACIDS FOR THE PASSIVATION OF PEROVSKITE SURFACE DEFECTS

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As fossil fuel reserves continue to decline, climate change intensifies, and the global demand for energy rapidly increases, the development of energy-efficient and renewable-energy-based technologies has become one of the greatest challenges in modern science [1]. Solar energy is particularly promising - within a single second, the Sun emits enough energy to theoretically meet humanity's energy needs for nearly one million years. These facts encourage researchers to develop new devices capable of efficiently converting solar radiation into electrical energy.

Over the past 15 years, thanks to extensive scientific research, perovskite solar cells (PSCs) have achieved efficiencies exceeding 27% [2]. Despite significant progress, there remain fundamental issues that must be addressed in science laboratories. One such issue is the presence of perovskite surface defects, (e.g. uncoordinated lead), which reduce device stability and limit efficiency [3]. Surface defects in PSCs are often passivated using relatively small organic molecules bearing functional groups (e.g., carboxylic acid, phosphonic acid, quaternary ammonium, etc.) that can form bonds with uncoordinated lead atoms [4]. Although the scientific literature contains numerous examples of materials used to reduce perovskite surface defects, there is still insufficient clarity regarding which functional group and molecular structure can deliver the best performance.

In this work various carbazole carboxylic acids were synthesized in order to investigate the influence of factors such as modifications in the carbazole core, distance between acid functional group and carbazole fragment on the interactions between the aromatic acids and perovskite surface defects. Nuclear magnetic resonance (NMR) experiments showed that interactions between PbI₂ and carbazole carboxylic acids are selective and depend on the structure of the aromatic acid.

[1] N. Wunderling and A. S. von der Heydt, Climate tipping point interactions and cascades: a review, *Earth System Dynamics*, vol. 15, pp. 41–74, 2024.

[2] Z. Xiong, Q. Zhang, K. Cai, H. Zhou, Q. Song, Z. Han, S. Kang, Y. Li, Q. Jiang, X. Zhang, and J. You, Homogenized chlorine distribution for >27% power conversion efficiency in perovskite solar cells, *Science*, vol. 390, pp. 638–642, 2025.

[3] D. B. Khadka, Y. Shirai, M. Yanagida, H. Ota, A. Lyalin, T. Taketsugu, and K. Miyano, Defect passivation in methylammonium/bromine-free inverted perovskite solar cells using charge-modulated molecular bonding, *Nature Communications*, vol. 15, art. no. 882, 2024.

[4] Y. Deng, X. Li, and R. Wang, Carboxyl functional group-assisted defects passivation strategy for efficient air-processed perovskite solar cells with excellent ambient stability, *Solar Energy Materials and Solar Cells*, vol. 230, art. no. 111242, 2021.