Combining Component Screening, Machine Learning and Molecular Engineering for the Design of High-Performance Inverted Perovskite Solar Cells

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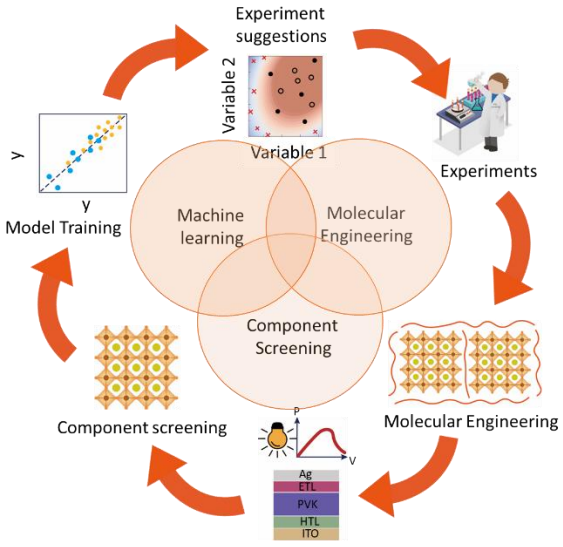
Abstract

Achieving high-performance inverted perovskite solar cells (PSCs) still remains a significant challenge, necessitating innovative approaches in materials selection and manufacturing technique optimization of perovskites. In this work, we unveil a paradigm shift in PSCs optimization. Through a judicious selection from a repertoire of 60 perovskite variants, we identified a composition with exemplary optical, thermal and electrical stability. Employing Bayesian machine learning, we navigated a labyrinth of over 1 billion process conditions, culminating in a record-breaking efficiency within a mere 80 iterations. Finally, the integration of bespoke in-situ polymerized ionic molecules allowed us to further augment performance of inverted PSCs, reaching an unparalleled power conversion efficiency of 25.76% (certified at 25.21%). The PSCs retained 94% of the initial efficiency after continuous operation in nitrogen atmosphere at 65 °C for 1920 hours. This work not only redefines the benchmarks for PSCs but also illuminates the path forward for photovoltaic innovations.



Reference

- B. Zhang, H. Zeng, H. Yin, D. Zheng, Z. Wan, C. Jia, T. Stuyver, J. Luo, Th. Pauporté, Combining Machine Learning, Component Screening and Molecular Engineering for the Design of High-Performance and Stable Inverted Perovskite Solar Cells. *Energy Environ. Sci*. **2024**, *17*, 5532 – 5541.