Reinforcement Learning for Configurational Design of High-PCE Chalcogenide Photo-Absorbers

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The configurational design of photovoltaic materials through alloying is one of the crucial techniques for achieving their highest potentials in solar energy conversion. However, the synergy of elements within the alloyed crystal often correlates strongly with its configurational site occupancies of constituent elements. In this work, we test Bayesian optimisation (BO), genetic algorithms (GA), and reinforcement learning (RL) as strategies for optimising photovoltaic materials. We show that reinforcement learning (RL) provides a flexible, interpretable and efficient framework for such optimizations. Focusing on three types of alloyed chalcogenide photo absorbers – the chalcogenide perovskites $BaZr(S,Se)_3$, the rocksalt $AgBiS_2$ and the Kesterite $(Cu,Ag)_2ZnSnS_4$, our trained RL models employing A2C[1] and PPO[2] policy learning strategies, showed higher learning capacity and smaller performance variance compared to the BO and GA models. Besides, the interpretability of our RL models allows insights into material configurations by analysing learned action probabilities. Benefitting from the fine-tunable parameters of neural networks, we envision that the transfer of simulation-based RL models to real experiments will hold an important role in future automated laboratories.

References

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[2] John Schulman, Filip Wolski, Prafulla Dhariwal, Alec Radford, Oleg Klimov, https://doi.org/10.48550/arXiv.1707.06347.

Figures

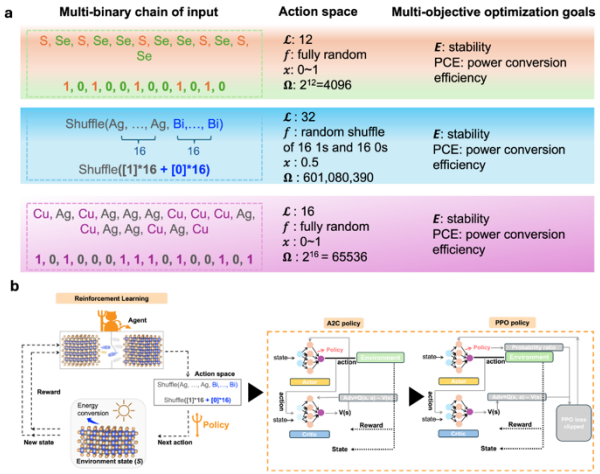

Figure 1. The materials design space and the reinforcement learning mechanism.