

Effect of Lewis Base Strength on Passivation of Perovskite Solar Cells

Andre Cook¹, Tim Jones², Noel Duffy,³ Scott Donne¹ and Greg Wilson²

¹*University of Newcastle, Callaghan, NSW 2308, Australia*

²*CSIRO Energy, Mayfield West, NSW 2304, Australia.*

³*CSIRO Energy Clayton Laboratories, Clayton, Vic 3169, Australia.*

E-mail: andre.cook@uon.edu.au

Organometal halide perovskite solar cells have recently shown the highest efficiency for a thin film device. This, combined with their tuneable adsorption spectrums make them ideal candidates for the top cells in tandem perovskite-silicon solar cells.¹ However, ion vacancies, or traps, on the perovskite surface inhibit charge transfer to the collection layers and accelerate degradation.² It is thought that these traps primarily form due to halide vacancies, leaving a positively charged surface on the perovskite.³ The individual vacancies can trap charge carriers, while collectively the positive surface could repel holes from the perovskite-hole collector interface. Electron-donating molecular Lewis bases have shown great efficacy in passivating these traps and can change the surface potential of the perovskite.⁴⁻⁶

Studies into passivation molecules usually investigate a limited number of molecules and use different methods to passivate different perovskite blends. This makes comparisons of treatments difficult, hindering our understanding of the passivation requirements and even the exact chemical nature of the traps. To address this problem we have passivated perovskite surfaces using a range of pyridine derivatives with ortho-substituted electron withdrawing or donating groups (Figure 1). This series changes the Lewis basicity of the binding pyridine group, whilst minimising steric effects. Morphology and surface charge measurements are performed using atomic force microscopy. Steady state and time resolved photoluminescence spectroscopy is used to identify the performance enhancement of the films. The effect of these treatments on device performance is also investigated. This study will provide new insight into the nature of the traps arising from under-coordinated surface Lewis-acid, and assist guiding the rational design of molecular agents.

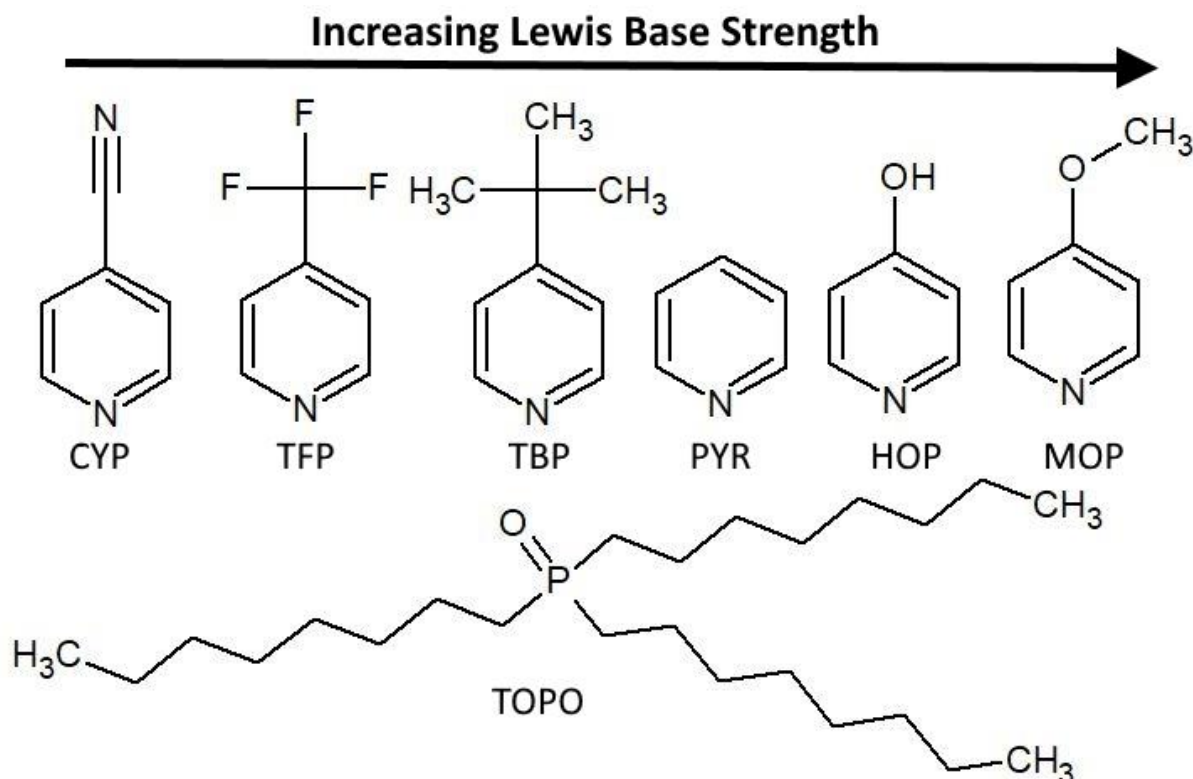


Figure 1. The functionalized pyridine Lewis bases used in this study along with tri-octylphosphine oxide (TOPO).

References

1. K. A. Bush, A. F. Palmstrom, J. Y. Zhengshan, M. Boccard, R. Cheacharoen, J. P. Mailoa, D. P. McMeekin, R. L. Hoyer, C. D. Bailie and T. Leijtens, 2017, 23.6%-efficient monolithic perovskite/silicon tandem solar cells with improved stability, *Nature Energy*, 2, 17009.
2. S. P. Sarmah, V. M. Burlakov, E. Yengel, B. Murali, E. Alarousu, A. M. El-Zohry, C. Yang, M. S. Alias, A. A. Zhumeckenov and M. I. Saidaminov, 2017, Double Charged Surface Layers in Lead Halide Perovskite Crystals, *Nano Letters*, 17, 2021-2027.
3. N. K. Noel, A. Abate, S. D. Stranks, E. S. Parrott, V. M. Burlakov, A. Goriely and H. J. Snaith, 2014, Enhanced photoluminescence and solar cell performance via Lewis base passivation of organic-inorganic lead halide perovskites, *ACS nano*, 8, 9815-9821.
4. R. J. Stewart, C. Grieco, A. V. Larsen, J. J. Maier and J. B. Asbury, 2016, Approaching Bulk Carrier Dynamics in Organo-Halide Perovskite Nanocrystalline Films by Surface Passivation, *The journal of physical chemistry letters*, 7, 1148-1153.
5. D. Song, D. Wei, P. Cui, M. Li, Z. Duan, T. Wang, J. Ji, Y. Li, J. M. Mbengue and Y. Li, 2016, Dual function interfacial layer for highly efficient and stable lead halide perovskite solar cells, *Journal of Materials Chemistry A*, 4, 6091-6097.
6. D. W. deQuilettes, S. Koch, S. Burke, R. Paranjli, A. J. Shropshire, M. E. Ziffer and D. S. Ginger, 2016, Photoluminescence Lifetimes Exceeding 8 μ s and Quantum Yields Exceeding 30% in Hybrid Perovskite Thin Films by Ligand Passivation, *ACS Energy Letters*.