Publications relating to hybrid halide perovskite solar cells from the Walsh Materials Design (WMD) research group

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Reviews and Perspectives

1. Butler, K. T., Frost, J. M. & Walsh, A. Ferroelectric materials for solar energy conversion: photoferroics revisited. *Energy Environ. Sci.* **8,** 838–848 (2015).

2. Walsh, A. Principles of chemical bonding and band gap engineering in hybrid organic–inorganic halide perovskites. *J. Phys. Chem. C* **119,** 5755–5760 (2015).

3. Frost, J. M. & Walsh, A. What is moving in hybrid halide perovskite solar cells? *Acc. Chem. Res.* **58,** 528–535 (2015).

Electronic Structure and Optical Properties

4. Brivio, F., Walker, A. B. & Walsh, A. Structural and electronic properties of hybrid perovskites for high-efficiency thin-film photovoltaics from first-principles. *APL Mater.* **1,** 042111 (2013).

5. Brivio, F., Butler, K. T., Walsh, A. & Van Schilfgaarde, M. Relativistic quasiparticle self-consistent electronic structure of hybrid halide perovskite photovoltaic absorbers. *Phys. Rev. B - Condens. Matter Mater. Phys.* **89,** 155204 (2014).

6. Leguy, A. *et al.* Experimental and theoretical optical properties of methylammonium lead halide perovskites. *Nanoscale* **8**, 6317 - 6327 (2016).

Molecular Disorder and Ferroelectricity

7. Frost, J. M. *et al.* Atomistic origins of high-performance in hybrid halide perovskite solar cells. *Nano Lett.* **14,** 2584–2590 (2014).

8. Frost, J. M., Butler, K. T. & Walsh, A. Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. *APL Mater.* **2,** 081506 (2014).

9. Weller, M. T., Weber, O. J., Frost, J. M. & Walsh, A. Cubic perovskite structure of black formamidinium lead iodide, α-$[HC(NH_2)_2]PbI_3$, at 298 K. *J. Phys. Chem. Lett.* **6,** 3209–3212 (2015).

10. Leguy, A. M. A. *et al.* The dynamics of methylammonium ions in hybrid organic-inorganic perovskite solar cells. *Nat. Commun.* **6,** 7124 (2015).

11. Grancini, G. *et al.* Role of microstructure in the electron–hole interaction of hybrid lead halide perovskites. *Nat. Photonics* **7,** 695 (2015).

12. Bakulin, A. A. *et al.* Real-time observation of organic cation reorientation in methylammonium lead-iodide perovskites. *J. Phys. Chem. Lett.* **6,** 3663–3669 (2015).

Defect Chemistry, Alloys & Ion Transport

13. Eames, C. *et al.* Ionic transport in hybrid lead iodide perovskite solar cells. *Nat. Commun.* **6,** 7497 (2015).

14. Walsh, A., Scanlon, D. O., Chen, S., Gong, X. G. & Wei, S.-H. Self-regulation mechanism for charged point defects in hybrid-halide perovskites. *Angew. Chemie Int. Ed.* **54,** 1791–1794 (2015).

15. Brivio, F., Caetano, C. & Walsh, A. Thermodynamic Origin of Photoinstability in the $CH_3NH_3Pb(I_{1-x}Br_x)_3$ Hybrid Halide Perovskite Alloy. *J. Phys. Chem. Lett.* **7**, 1083 – 1087 (2016).

Phonons and Vibrational Spectra

16. Brivio, F. *et al.* Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide. *Phys. Rev. B* **92,** 144308 (2015).

Solar Cells and Contacts

17. Murray, A. *et al.* Modular design of SPIRO-OMeTAD analogues as hole transport materials in solar cells. *Chem. Commun.* **51,** 8935–8938 (2015).

18. Butler, K. T., Frost, J. M. & Walsh, A. Band alignment of the hybrid halide perovskites $CH_3NH_3PbCl_3$, $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$. *Mater. Horiz.* **2,** 228–231 (2015).

19. Butler, K. T., Kumagai, Y., Oba, F. & Walsh, A. Screening procedure for structurally and electronically matched contact layers for high-performance solar cells: hybrid perovskites. *J. Mater. Chem. C* **4,** 1149–1158 (2016).

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20. da Silva, E. L., Skelton, J. M., Parker, S. C. & Walsh, A. Phase stability and transformations in the halide perovskite $CsSnI_3$. *Phys. Rev. B* **91,** 144107 (2015).

21. Protesescu, L. *et al.* Nanocrystals of Cesium Lead Halide Perovskites ($CsPbX_3$, X = Cl, Br, and I): Novel Optoelectronic Materials Showing Bright Emission with Wide Color Gamut. *Nano Lett.* **15,** 3692–3696 (2015).

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22. Yang, R. X., Butler, K. T. & Walsh, A. Assessment of Hybrid Organic-Inorganic Antimony Sulfides for Earth-Abundant Photovoltaic Applications. *J. Phys. Chem. Lett.* **6,** 5009–5014 (2015).

23. Ganose, A. M., Butler, K. T., Walsh, A. & Scanlon, D. O. Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. *J. Mater. Chem. A* **4,** 2060–2068 (2016).

24. Butler, K. T.; Mckechnie, S.; Azarhoosh, P.; van Schilfgaarde, M.; Scanlon, D. O.; Walsh, A. Quasi-Particle Electronic Band Structure and Alignment of the V-VI-VII Semiconductors SbSI, SbSBr, and SbSeI for Solar Cells. *Appl. Phys. Lett.* **2016**, *108*, 112103.