Benjamin A. D. Williamson MSci, PhD, MRSC, NKS

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Employment

Norwegian University of Science and Technology (NTNU) (2019 - Present)

Trondheim, Norway

Postdoctoral Researcher in Computational Materials Design

Functional Materials and Materials Chemistry Research Group (FACET)

Advisor: Prof. Sverre M. Selbach

University College London (2018 – 2019)

London, United Kingdom

Postdoctoral Research Associate in Computational Materials Design

Scanlon Materials Theory Group Advisor: Prof. David O. Scanlon

University Education

University College London (2014 - 2018)

London, United Kingdom

PhD in Computational Inorganic Materials Chemistry

Thesis title: Understanding the Electronic and Thermodynamic Properties of Wide Band Gap Materials

Supervisor: Prof. David O. Scanlon; Secondary Supervisor: Prof. Claire J. Carmalt

University College London (2010 – 2014)

London, United Kingdom

MSci in Chemistry – 1st Class Honours

MSci dissertation title: Computational Design of Next-Generation p-Type Semiconductors

Supervisor: Prof. David O. Scanlon

Publications

(In reverse chronological order)

1. Experimental and theoretical study of the electronic structures of lanthanide indium perovskites $LnInO_3$

P. Hartley, K.H.L. Zhang, M.V. Hohmann, L.F.J. Piper, D.J. Morgan, R.G. Edgell, D.O. Scanlon, **B.A.D. Williamson**, and A. Regoutz; *J. Phys. Chem. C*, 125, 6387, (2021)

2. Photocatalytic, Structural and Optical Properties of Mixed Anion Solid Solutions $Ba_3Sc_{2-x}In_xCu_2S_2$ and $Ba_3In_2O_5Cu_2S_{2-y}Se_y$

G. Limburn, M. Stephens, **B.A.D. Williamson**, A. Iborra-Torres, D.O. Scanlon and G. Hyett; *J. Mater. Chem. A*, 8, 19887-19897 (2020)

DOI: 10.1039/D0TA06629J

3. Computationally Driven Discovery of Layered Quinary Oxychalcogendides: Potential p-Type Transparent Conductors?

B.A.D. Williamson, G.J. Limburn, G. Hyett, G. W. Watson and D.O. Scanlon; *Matter, Cell Press*, 3,3, 759-781 (2020)

DOI: 10.1016/j.matt.2020.05.020

Article Preview by A. Walsh and J-S. Park: The Holey Grail of Transparent Electronics DOI: 10.1016/j.matt.2020.08.008

4. Computational Prediction of the Thermoelectric Performance of LaZnOPn (Pn = P, As) M. Einhorn, **B.A.D. Williamson** and D.O. Scanlon; *J. Mater. Chem. A*, 8, 7914-7924 (2020) DOI: 10.1039/D0TA00690D

5. Resonant Ta Doping for Enhanced Mobility in Transparent Conducting SnO₂

B.A.D. Williamson, T.J. Featherstone, S. Sathasivam, J.E.N Swallow, H. Shiel, L.A.H. Jones, M.J. Smiles, A. Regoutz, T-L. Lee, X. Xia, C. Blackman, P.K. Thakur, C.J. Carmalt, I.P. Parkin, T.D. Veal and D.O. Scanlon; Chem. Mater., 32, 5, 1964-1973 (2020)

DOI: 10.1021/acs.chemmater.9b04845

Work featured on the front cover

6. Enhanced Photocatalytic and Antibacterial Ability of Cu-doped Anatase TiO₂ Thin Films: Theory and **Experiment**

A.M. Alotaibi, B.A.D. Williamson, S. Sathasivam, A. Kafizas, M. Alqahtani, C. Sotelo-Vazquez, J. Buckeridge, J. Wu, S.P. Nair, D.O. Scanlon and I.P. Parkin; ACS Appl. Mater. Interfaces just accepted manuscripts (2020)

DOI: 10.1021/acsami.9b22056

7. Resonant Doping for High Mobility Transparent Conductors: The Case of Mo-doped In₂O₃ J.E.N. Swallow, B.A.D. Williamson, S. Sathasivam, M. Birkett, T.J. Featherstone, P.A.E. Murgatroyd, H.J. Edwards, Z.W. Lebens-Higgins, D.A. Duncan, M. Farnworth, P. Warren, N. Peng, T-L. Lee, L.F.J. Piper, A. Regoutz, C.J. Carmalt, I.P.Parkin, V.R. Dhanak, D.O. Scanlon and T.D. Veal; Mater. Horiz., 7, 236-243 (2020)

DOI: 10.1039/C9MH01014A

8. Dispelling the Myth of Passivated Codoping in TiO₂

B.A.D. Williamson, J. Buckeridge, N.P. Chadwick, S. Sathasivam, C.J. Carmalt, I.P. Parkin and D.O. Scanlon; Chem. Mater., 31 (7), 2577-2589 (2019)

DOI: 10.1021/acs.chemmater.9b00257

9. Origin of High-Efficiency Photoelectrochemical Water Splitting on Hematite/Functional Nanohybrid Metal Oxide Overlayer Photoanode after a Low Temperature Inert Gas Annealing Treatment S. Ho-Kimura, B.A.D. Williamson, S. Sathasivam, S.J.A. Moniz, G. He, W. Luo, D.O. Scanlon, J. Tang, I.P. Parkin; ACS Omega, 4 (1), 1449-1459 (2019) DOI: 10.1021/acsomega.8b02444

10. Phosphorus Doped SnO₂ Thin Films for Transparent Conducting Oxide Applications: Synthesis, Optoelectronic Properties and Computational Models

M.J. Powell, B.A.D. Williamson, S-Y. Baek, J. Manzi, D. Potter, D.O. Scanlon and C.J. Carmalt; Chem. Sci., 9 (41), 7968-7980 (2018)

DOI: 10.1039/C8SC02152J

11. Enhanced Electrical Properties of Antimony Doped Tin Oxide Thin Films Deposited via Aerosol Assisted Chemical Vapour Deposition

S. Ponja, B.A.D. Williamson, S. Sathasivam, D.O. Scanlon, I.P. Parkin, C.J. Carmalt; J. Mater. Chem. C, 6, 7257-7266 (2018)

DOI: 10.1039/C8TC01929K

12. A Novel Laboratory-based Hard X-ray Photoelectron Spectroscopy System

A. Regoutz, M. Mascheck, T. Wiell, S.K. Eriksson, C. Liljenberg, K. Tetzner, B.A.D. Williamson, D. O. Scanlon and P. Palmgren; *Rev. Sci. Inst.*, 89 (7), 073105 (2018)

DOI: 10.1063/1.5039829

Chemical Vapor Deposition of Photocatalytically Active Pure Brookite TiO₂ Thin Films
 A.M. Alotaibi, S. Sathasivam , B.A.D. Williamson, A. Kafizas , C. Sotelo-Vazquez, A. Taylor, D.O. Scanlon, and I.P. Parkin; Chem. Mater., 30 (4), 1353-1361 (2018)
 DOI: 10.1021/acs.chemmater.7b04944

14. A Deeper Understanding of Interstitial Boron-Doped Anatase Thin Films as A Multifunctional Layer Through Theory and Experiment

M. Quesada-Gonzalez, **B.A.D. Williamson**, C. Sotelo-Vazquez, A. Kafizas, N.D. Boscher, R. Quesada-Cabrera, D.O. Scanlon, C.J. Carmalt, I.P. Parkin; *J. Phys. Chem. C*, 122 (1), 714-726 (2018)

DOI: 10.1021/acs.jpcc.7b11142

15. Self-Compensation in Transparent Conducting F-Doped SnO₂

J.E.N. Swallow, **B.A.D. Williamson**, T.J. Whittles, M. Birkett, T.J. Featherstone, N. Peng, A. Abbott, M. Farnworth, K.J. Cheetham, P. Warren, D.O. Scanlon, V.R. Dhanak, T.D.Veal; *Adv. Funct. Mater.*, 1701900 (2017)

DOI: 10.1002/adfm.201701900

16. Chemical Vapor Deposition Synthesis and Optical Properties of Nb_2O_5 Thin Films with Hybrid Functional Theoretical Insight into Band Structure and Band Gaps

S. Sathasivam, **B.A.D. Williamson**, S.A. Al Thabaiti, A.Y. Obaid, S.N. Basahel, M. Mokhtar, D.O. Scanlon, C.J. Carmalt, I.P.Parkin; *ACS Appl. Mater. Interfaces*, 9 (21), 18031-18038 (2017) DOI: 10.1021/acsami.7b00907

17. Computational and Experimental Study of Ta₂O₅ Thin Films

S. Sathasivam, **B.A.D. Williamson**, A. Kafizas, S.A. Althabaiti, A.Y. Obaid, S.N. Basahel, D.O. Scanlon, C.J. Carmalt, I.P Parkin; *J. Phys. Chem. C*, 121 (1), 202-210 (2017) DOI: 10.1021/acs.jpcc.6b11073

18. Transparent Conducting n-type ZnO:Sc – Synthesis, Optoelectronic Properties and Theoretical Insight S.C. Dixon, S. Sathasivam, **B.A.D. Williamson**, D.O. Scanlon, C.J. Carmalt, I.P. Parkin; J. Mater. Chem. C, 5, 7585-7597 (2017)

DOI: 10.1039/C7TC02389H

19. Engineering Valence Band Dispersion for High Mobility p-Type Semiconductors

B.A.D. Williamson, J. Buckeridge, J. Brown, S. Ansbro, R.G. Palgrave, D.O. Scanlon; *Chem. Mater.*, 29 (6), 2402-2413 (2017)

DOI: 10.1021/acs.chemmater.6b03306

Work featured as part of the front cover

20. A Single-Source Precursor Approach to Solution Processed Indium Arsenide Thin Films

P. Marchand, S. Sathasivam, **B.A.D. Williamson**, D. Pugh, S.M. Bawaked, S.N. Basahel, A.Y. Obaid, D.O. Scanlon, I.P. Parkin, C.J. Carmalt; *J. Mater. Chem. C*, 4, 6761-6768 (2016)

DOI: 10.1039/C6TC02293F

In Submission

21. *ABWCX a Promising n-Type Thermoelectric Oxide with the DEYFZ Crystal Structure* K.B. Spooner, A.M. Ganose, W.W.W.Leung, J.Buckeridge, **B.A.D. Williamson**, R.G. Palgrave, and D.O. Scanlon, ?, *in submission*

22. Benchmarking the quantitative and qualitative performance of point defect calculations in semiconductors with semi-local DFT

D. Broberg, K. Bystrom, S. Srivastava, D. Dahliah, N. Adamski, **B.A.D. Willamson**, A. Rowberg, L. Weston, M. Turiansky, D.O. Scanlon, C.G. Van de Walle, S. Dwaraknath, J.B. Varley, K. Persson, M. Asta and G. Hautier; *in submission*

- 23. Resonant XX Doping for High-Mobility In_2O_3 -Based Conductors with Enhanced Near-Infrared Transparency
 - T. J. Featherstone, J. Willis, J.E.N. Swallow, **B.A.D. Williamson**, L.A.H. Jones, T.-Li. Lee, P.K. Thakur, G.W. Watson, T. Koida, D.O. Scanlon, and T.D. Veal; *in submission*
- 24. Effect of pseudo-cubic (111)-oriented orthorhombic substrate facets on perovskite oxide thin film synthesis
 - K. Kjærnes, T. Bolstad, D.M. Evans, E. Lysne, **B.A.D. Williamson**, D. Meier, S.M. Selbach, T. Tybell; *in submission*

Conference Presentations

- 1. Contributed: B.A.D Williamson: *Computational discovery of an earth abundant, stable Li solid electrolyte*, FACET Sustainability Workshop, Trondheim, Norway 2021 –Oral
- 2. Contributed: B.A.D Williamson: *Computational Insights into Li diffusion in Solid State Electrolytes*, 7th Inorganic and Materials Norsk Kjemisk Selskap (NKS) Meeting, Værnes, Norway 2020 –Oral
- 3. Contributed: B.A.D Williamson: Resonant Doping for High Mobility Transparent Conductors: The Case of Mo-doped In_2O_3 , 11th Petite Workshop on defects in energy materials; Sommarøy, Norway 2019 Oral
- 4. Contributed: B.A.D Williamson: Computationally Aided Discovery of Layered Quinary Oxychalcogenide p-type Transparent Conductor, Workshop For Atomistic Modelling; Trondheim, Norway 2019 Poster
- 5. Contributed: B.A.D Williamson: Dispelling the Myth of Passivated Codoping in TiO_2 , MRS Fall Meeting; Boston US, 2018 Oral
- 6. Contributed: B.A.D.Williamson: Computationally Aided Discovery of Layered Quinary Oxychalcogenide p-type Transparent Conductors, MRS Fall Meeting; Boston US, 2018 Poster Winner of the ICDD prize for materials characterisation
- 7. Contributed: B.A.D Williamson: *Doubled Conductivity in Transparent Conducting In*₂O₃ *Through Novel Dopant Design*, MMM Hub; Thomas Young Centre, London, UK, 2018 Poster
- 8. Invited: B.A.D Williamson: *Doubled Conductivity in Transparent Conducting In*₂O₃ *Through Novel Dopant Design*, MCC 3rd Conference, Lincoln UK, 2018 Oral
- 9. Contributed: B.A.D Williamson: Doubled Conductivity in Transparent Conducting In_2O_3 Through Novel Dopant Design, Gordon Research Conference; Defects In Semiconductors, Colby-Sawyer College, New Hampshire, US, 2018 Poster
- 10. Invited: B.A.D Williamson: *Beyond Conventional Doping in SnO*₂, Thomas Young Centre, London UK, 2017 Oral
- 11. Contributed: B.A.D Williamson: *Beyond Conventional Doping in SnO*₂, E-MRS; Spring Meeting, Strasbourg France, 2017 Poster
- 12. Contributed: B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, E-MRS; Spring Meeting, Strasbourg France, 2017 Oral
- 13. Contributed: B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, MRS Fall Meeting; Boston US, 2016 Poster
- 14. Contributed: B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, SSCG Christmas Meeting; Canterbury UK, 2015 Poster

Industrial Collaborations

2014 – 2019: Pilkingtons NSG Group (www.pilkington.com)

2021: Equinor (www.equinor.com)

Teaching

2021: Lecturer of Masters Course "TMT4245 Functional Materials" at NTNU

2019 – Present: Supervised 4 final year Masters research projects at NTNU 2014 – 2019: Supervised six final year MSci research projects at UCL 2014 – 2019: Demonstrated in 1st year workshops (CHEM1004)

2018 – 2019: Tutor in 1st year inorganic chemistry courses at UCL (CHEM1101 and CHEM0013)

References

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