

# 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 – 1<sup>st</sup> Class Honours

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

Supervisor: Prof. David O. Scanlon

### Publications

(In reverse chronological order)

1. *Mesophase transition in  $[(C_2H_5)N][FeBrCl_3]$  and  $[(CH_3)_4N][FeBrCl_3]$  ferroic plastic crystals*  
J. Walker, K. P. Marshall, **B.A.D. Williamson**, J.S. Beceiro, N. S. Løndal, S. M. Selbach, S. C. Garcia, D. Chernyshov, M-A. Einarsrud; *Chem. Mater.*, just accepted, (2021)
2. *Ligand field-induced exotic electronic state of a transition metal dopant for an infrared transparent conductive oxide: A-doped  $BC_2$*   
M. Fukumoto, Y. Hirose, **B.A.D. Williamson**, S. Nakao, K. Kimura, K. Hayashi, Y. Sugisawa, D. Sekiba, D.O. Scanlon and T. Hasegawa; *Adv. Func. Mater.*, just accepted, (2021)
3.  *$BaBi_2O_6$ : A Promising n-Type Thermoelectric Oxide with the  $PbSb_2O_6$  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, *Chem. Mater.*, <https://pubs.acs.org/doi/10.1021/acs.jpcc.0c11592>, (2021)  
DOI: 10.1021/acs.chemmater.1c02164
4. *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)  
DOI: 10.1021/acs.jpcc.0c11592
5. *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
  6. *Computationally Driven Discovery of Layered Quinary Oxychalcogenides: 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
  7. *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
  8. *Resonant Ta Doping for Enhanced Mobility in Transparent Conducting  $SnO_2$*   
**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](#)
  9. *Enhanced Photocatalytic and Antibacterial Ability of Cu-doped Anatase  $TiO_2$  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
  10. *Resonant Doping for High Mobility Transparent Conductors: The Case of Mo-doped  $In_2O_3$*   
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
  11. *Dispelling the Myth of Passivated Codoping in  $TiO_2$*   
**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
  12. *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
  13. *Phosphorus Doped  $SnO_2$  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
14. *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
  15. *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
  16. *Chemical Vapor Deposition of Photocatalytically Active Pure Brookite TiO<sub>2</sub> 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
  17. *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
  18. *Self-Compensation in Transparent Conducting F-Doped SnO<sub>2</sub>*  
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
  19. *Chemical Vapor Deposition Synthesis and Optical Properties of Nb<sub>2</sub>O<sub>5</sub> 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
  20. *Computational and Experimental Study of Ta<sub>2</sub>O<sub>5</sub> 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
  21. *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
  22. *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](#)
  23. *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*

24. *Tuning the Thermoelectric Performance of ABO<sub>3</sub>-based ceramics by controlled exsolution and microstructuring*  
N. Kanas, **B.A.D. Williamson**, F. Steinbach, R. Hinterding, M-A. Einarsrud, S.M. Selbach, A. Feldhoff and K. Wiik; *in submission*
25. *Investigation of factors affecting the stability of compounds formed by isovalent substitution in layered coinage metal chalcogenides leading to identification of Ba<sub>3</sub>Sc<sub>2</sub>O<sub>5</sub>Cu<sub>2</sub>Se<sub>2</sub>, Ba<sub>3</sub>Y<sub>2</sub>O<sub>5</sub>Cu<sub>2</sub>S, Ba<sub>3</sub>Sc<sub>2</sub>O<sub>5</sub>Ag<sub>2</sub>Se<sub>2</sub>, and Ba<sub>3</sub>In<sub>2</sub>O<sub>5</sub>Ag<sub>2</sub>Se<sub>2</sub>*  
G.J. Limburn, D.W. Davies, N. Langridge, Z. Malik, **B.A.D. Williamson**, D.O. Scanlon, and G. Hyett; *in submission*
26. *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. Williamson**, 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*
27. *Resonant XX Doping for High-Mobility In<sub>2</sub>O<sub>3</sub>-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*
28. *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<sub>2</sub>O<sub>3</sub>*, 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<sub>2</sub>*, 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<sub>2</sub>O<sub>3</sub> 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<sub>2</sub>O<sub>3</sub> Through Novel Dopant Design*, MCC 3rd Conference, Lincoln UK, 2018 – Oral

9. Contributed: B.A.D Williamson: *Doubled Conductivity in Transparent Conducting In<sub>2</sub>O<sub>3</sub> 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<sub>2</sub>*, Thomas Young Centre, London UK, 2017 – Oral
11. Contributed: B.A.D Williamson: *Beyond Conventional Doping in SnO<sub>2</sub>*, 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](http://www.pilkington.com))  
 2021 – Present: Equinor ([www.equinor.com](http://www.equinor.com))  
 Northern Lights ([www.northernlightsccs.com](http://www.northernlightsccs.com))  
 Total Energies ([www.totalenergies.com](http://www.totalenergies.com))  
 Shell ([www.shell.com](http://www.shell.com))

## Teaching

2021: Lecturer of Masters Course "TMT4245 FUNCTIONAL MATERIALS" at NTNU  
 2019 – Present: Supervised five final year Masters research projects at NTNU  
 2014 – 2019: Supervised six final year MSci research projects at UCL  
 2014 – 2019: Demonstrated in 1<sup>st</sup> year workshops (CHEM1004)  
 2018 – 2019: Tutor in 1<sup>st</sup> year inorganic chemistry courses at UCL (CHEM1101 and CHEM0013)

## References

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