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

Email: benjamin.williamson@ntnu.no
(Previous Email: benjamin.williamson.10@ucl.ac.uk)
Website: badw.github.io

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, just accepted*, (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

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. 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*

22. 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*

23. 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 Insights into Li diffusion in Solid State Electrolytes*, 7th Inorganic and Materials Norsk Kjemisk Selskap (NKS) Meeting, Værnes, Norway 2020 –Oral
- 2. 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
- 3. Contributed: B.A.D Williamson: Computationally Aided Discovery of Layered Quinary Oxychalcogenide p-type Transparent Conductor, Workshop For Atomistic Modelling; Trondheim, Norway 2019 Poster
- 4. Contributed: B.A.D Williamson: *Dispelling the Myth of Passivated Codoping in TiO*₂, MRS Fall Meeting; Boston US, 2018 Oral
- 5. 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
- 6. 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
- 7. Invited: B.A.D Williamson: *Doubled Conductivity in Transparent Conducting In*₂O₃ *Through Novel Dopant Design*, MCC 3rd Conference, Lincoln UK, 2018 Oral
- 8. 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
- 9. Invited: B.A.D Williamson: *Beyond Conventional Doping in SnO*₂, Thomas Young Centre, London UK, 2017 Oral
- 10. Contributed: B.A.D Williamson: Beyond Conventional Doping in SnO_2 , E-MRS; Spring Meeting, Strasbourg France, 2017 Poster
- 11. Contributed: B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, E-MRS; Spring Meeting, Strasbourg France, 2017 Oral
- 12. Contributed: B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, MRS Fall Meeting; Boston US, 2016 Poster
- 13. 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

Prof. David O. Scanlon University College London London WC1H 0AJ

Tel: (+44) 7943584620 Email: d.scanlon@ucl.ac.uk Prof. Sverre M. Selbach Norwegian University of Science and Technology Trondheim

Tel: (+47) 91646302 Email: selbach@ntnu.no