

# Dr Benjamin A. D. Williamson

## MSci MPhil PhD



Department of Materials Science and Engineering  
Norwegian University of Science and Technology (NTNU)  
7491 Trondheim  
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### 🏢 Employment

#### Norwegian University of Science and Technology (NTNU) (2019 – Present)

Trondheim, Norway

Researcher in Computational Materials Design

Themes: Battery materials, ferroelectrics/multiferroics, solar cells, novel inorganic/organic functional materials

Functional Materials and Materials Chemistry Research Group (FACET)

Advisors: Prof. Tor Grande & Prof. Sverre M. Selbach

#### University College London (2018 – 2019)

London, United Kingdom

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

MPhil/PhD in Computational Inorganic Materials Chemistry – *no corrections*

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

### 📖 Peer Reviewed Publications

As of July 2024:

Total Citations: 1252 (since 2017)

*h*-index: 18

(In reverse chronological order)

32. *Doping Implications of Li-ion Solid State Electrolyte Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub>*  
K. Eggstad, S. M. Selbach, and **B.A.D. Williamson**, *J. Mater. Chem. A*, Advance Article, (2024)  
DOI: 10.1039/D4TA01487A  
Work selected as one of the Journal of Materials Chemistry A HOT Papers 2024

31. *On the solubility of Bi in tetragonal tungsten bronzes*  
C. R. Zeiger; **B.A.D. Williamson**; J. Walker, M.-A. Einarsrud, T. Grande. *J. Euro. Ceram. Soc.*, 44, 6, 3723-3733 (2024)  
DOI: 10.1016/j.jeurceramsoc.2024.01.005
30. *The effect of cation size on structure and properties of Ba-based tetragonal tungsten bronzes  $Ba_4M_2Nb_{10}O_{30}$  ( $M = Na, K$  or  $Rb$ ) and  $Ba_4M_2Nb_8Ti_2O_{30}$  ( $M = Ca$  or  $Sr$ )*  
N. S. Løndal; **B.A.D. Williamson**; J. Walker, M.-A. Einarsrud, T. Grande. *Phys. Chem. Chem. Phys.*, 26, 3350-3366 (2024)  
DOI: 10.1039/D3CP05666J
29. *Oxygen absorption in nanocrystalline  $h\text{-RMnO}_3$  ( $R=Y, Ho, Dy$ ) and the effect of Ti donor doping*  
F. Danmo; **B.A.D. Williamson**; D. Småbråten, N. Gaukås, E.R. Østli, T. Grande; J. Glaum; S. Selbach; *Chem. Mater.*, 34, 15, 5764-5776 (2023)  
DOI: 10.1021/acs.chemmater.3c00189
28. *Multi-Phase Sputtered  $TiO_2$ -Induced Current–Voltage Distortion in  $Sb_2Se_3$  Solar Cells*  
C.H. Don, T.P. Shalvey, M.J. Smiles, L. Thomas, L.J. Phillips, T.D.C. Hobson, H. Finch, L.A.H. Jones, J.E.N. Swallow, N. Fleck, C. Markwell, P.K. Thakur, T.-L. Lee, D. Biswas, L. Bowen, **B.A.D. Williamson**, D.O. Scanlon, V.R. Dhanak, K. Durose, T.D. Veal, J.D. Major; *Adv. Mater. Int.*, 2300238 (2023)  
DOI: 10.1002/admi.202300238
27. *High-throughput calculations of charged point defect properties with semi-local density functional theory performance benchmarks for materials screening applications*  
D. Broberg, K. Bystrom, S. Srivastava, D. Dahliah, **B.A.D. Williamson**, L. Weston, D. O. Scanlon, G.-M. Rignanes, S. Dwaraknath, J. Varley, K. A. Persson, M. Asta, G. Hautier; *npj Comp. Mater.*, 9, 1, 72 (2023)  
DOI: 10.17188/mpcontributes/1907859
26. *Tuning the Thermoelectric Performance of  $CaMnO_3$ -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; *ACS Appl. Energy Mater.*, 5, 10, 12396–12407 (2022)  
DOI: 10.1021/acsaem.2c02012
25. *Computational Prediction and Experimental Realisation of Earth Abundant Transparent Conducting Oxide Gated  $ZnSb_2O_6$*   
A. J. Jackson, B. J. Parrett, J. Willis, A. M. Ganose, W. W. W. Leung, **B.A.D. Williamson**, Y. Liu, T. K. Kim, M. Hoesch, L. Ishibe-Veiga, R. Kalra, J. Neu, C. A. Schmuttenmaer, T.-L. Lee, A. Regoutz, T. D. Veal, R. G. Palgrave, R. Perry and D. O. Scanlon; *ACS Energy Lett.* 2022, 7, XXX, 3807–3816, (2022)  
DOI: 10.1021/acsenerylett.2c01961
24. *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.*, 34, 6, 2585-2598, (2022)  
DOI: 10.1021/acs.chemmater.1c03778
23. *Investigation of factors affecting the stability of compounds formed by isovalent substitution in layered oxychalcogenides, leading to identification of  $Ba_3Sc_2O_5Cu_2Se_2$ ,  $Ba_3Y_2O_5Cu_2S_2$ ,  $Ba_3Sc_2O_5Ag_2Se_2$  and  $Ba_3In_2O_5Ag_2Se_2$*   
G. J. Limburn, D. W. Davies, N. Langridge, Z. Malik, **B. A. D. Williamson**, D. O. Scanlon, and G. Hyett; *J. Mater. Chem. C*, 10, 3784-3795, (2022)  
DOI: 10.1039/D1TC05051F
22. *Ligand Field-Induced Exotic Dopant for Infrared Transparent Electrode: W in Rutile  $SnO_2$*   
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.*, 2110832, (2021)  
DOI: 10.1002/adfm.202110832
21.  *$BaBi_2O_6$ : 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>pted, 33, 7441, (2021)  
DOI: 10.1021/acs.chemmater.1c02164

20. *Experimental and theoretical study of the electronic structures of lanthanide indium perovskites  $\text{LnInO}_3$*   
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
19. *Photocatalytic, Structural and Optical Properties of Mixed Anion Solid Solutions  $\text{Ba}_3\text{Sc}_{2-x}\text{In}_x\text{Cu}_2\text{S}_2$  and  $\text{Ba}_3\text{In}_2\text{O}_5\text{Cu}_2\text{S}_{2-y}\text{Se}_y$*   
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
18. *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
17. *Computational Prediction of the Thermoelectric Performance of  $\text{LaZnOPn}$  ( $\text{Pn} = \text{P}, \text{As}$ )*  
M. Einhorn, **B.A.D. Williamson** and D.O. Scanlon; *J. Mater. Chem. A*, 8, 7914-7924 (2020)  
DOI: 10.1039/D0TA00690D
16. *Resonant Ta Doping for Enhanced Mobility in Transparent Conducting  $\text{SnO}_2$*   
**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
15. *Enhanced Photocatalytic and Antibacterial Ability of Cu-doped Anatase  $\text{TiO}_2$  Thin Films: Theory and Experiment*  
A.M. Alotaibi, **B.A.D. Williamson**, S. Sathasivam, A. Kafizas, M. Alqahtani, C. Sotelo-Vazquez, J. Buck-eridge, 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
14. *Resonant Doping for High Mobility Transparent Conductors: The Case of Mo-doped  $\text{In}_2\text{O}_3$*   
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
13. *Dispelling the Myth of Passivated Codoping in  $\text{TiO}_2$*   
**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 Overlay 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
11. *Phosphorus Doped  $\text{SnO}_2$  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
10. *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

9. *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
8. *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
7. *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
6. *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
5. *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
4. *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
3. *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
2. *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
1. *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*

3. *Mobile Point Defects for Conductive and Memristive Domain Walls in ABO<sub>3</sub>*  
K. Eggestad, **B.A.D. Williamson**, and S. M. Selbach, *in submission*
2. *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*
1. *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*

6 additional publications are currently in preparation

## Conference Presentations

1. **Contributed:** B.A.D Williamson: *Computational Analysis of a Promising Earth Abundant, Stable, Lithium Solid Electrolyte.*, MRS Spring, Seattle, USA 2024 – Talk
2. **Invited:** B.A.D Williamson: *Approaches to Overcoming the Challenges of Ab Initio Prediction of Functional Plastic Crystals.*, NMBU Advancing Functional Molecular Matter , NMBU, Ås, Norway 2024 – Talk
3. **Contributed:** B.A.D. Williamson *First Principles Insights into Phase Transitions, Disorder and Electronic Properties of Lead-Free Ba-based Tetragonal Tungsten Bronzes.*, IMF Ferroelectrics, Tel Aviv, Israel 2023 –Talk
4. **Contributed:** B.A.D. Williamson *Can we Utilise Phonons to Enhance Li-ion Diffusion?*, MRS Fall Meeting, Boston, USA 2022 –Talk
5. **Contributed:** B.A.D. Williamson *The Underlying Mechanisms of Ultrahigh Mobility in  $\text{Bi}_2\text{O}_2\text{Se}$  using Self-Consistent GW Method*, MRS Spring Meeting, Honolulu, USA 2022 –Talk
6. **Contributed:** B.A.D Williamson: *Computational discovery of an earth abundant, stable Li solid electrolyte*, FACET Sustainability Workshop, Trondheim, Norway 2021 –Talk
7. **Contributed:** B.A.D Williamson: *Computational discovery of an earth abundant, stable Li solid electrolyte*, FACET Sustainability Workshop, Trondheim, Norway 2021 –Talk
8. **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 –Talk
9. **Contributed:** B.A.D Williamson: *Resonant Doping for High Mobility Transparent Conductors: The Case of Mo-doped  $\text{In}_2\text{O}_3$* , 11th Petite Workshop on defects in energy materials; Sommarøy, Norway 2019 – Talk
10. **Contributed:** B.A.D Williamson: *Computationally Aided Discovery of Layered Quinary Oxychalcogenide p-type Transparent Conductor*, Workshop For Atomistic Modelling; Trondheim, Norway 2019 – Poster
11. **Contributed:** B.A.D Williamson: *Dispelling the Myth of Passivated Codoping in  $\text{TiO}_2$* , MRS Fall Meeting; Boston US, 2018 – Talk
12. **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**
13. **Contributed:** B.A.D Williamson: *Doubled Conductivity in Transparent Conducting  $\text{In}_2\text{O}_3$  Through Novel Dopant Design*, MMM Hub; Thomas Young Centre, London, UK, 2018 – Poster
14. **Invited:** B.A.D Williamson: *Doubled Conductivity in Transparent Conducting  $\text{In}_2\text{O}_3$  Through Novel Dopant Design*, MCC 3rd Conference, Lincoln UK, 2018 – Talk
15. **Contributed:** B.A.D Williamson: *Doubled Conductivity in Transparent Conducting  $\text{In}_2\text{O}_3$  Through Novel Dopant Design*, Gordon Research Conference; Defects In Semiconductors, Colby-Sawyer College, New Hampshire, US, 2018 – Poster
16. **Invited:** B.A.D Williamson: *Beyond Conventional Doping in  $\text{SnO}_2$* , Thomas Young Centre, London UK, 2017 – Talk
17. **Contributed:** B.A.D Williamson: *Beyond Conventional Doping in  $\text{SnO}_2$* , E-MRS; Spring Meeting, Strasbourg France, 2017 – Poster
18. **Contributed:** B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, E-MRS; Spring Meeting, Strasbourg France, 2017 – Talk
19. **Contributed:** B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, MRS Fall Meeting; Boston US, 2016 – Poster
20. **Contributed:** B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, SSCG Christmas Meeting; Canterbury UK, 2015 – Poster

## Industrial Collaborations

2023 – Present     Hydro ([www.hydro.com](http://www.hydro.com))  
2021 – Present:     Equinor ([www.equinor.com](http://www.equinor.com))  
                             Northern Lights ([www.northernlightscs.com](http://www.northernlightscs.com))  
                             Total Energies ([www.totalenergies.com](http://www.totalenergies.com))  
                             Shell ([www.shell.com](http://www.shell.com))  
2014 – 2019:       Pilkingtons NSG Group ([www.pilkington.com](http://www.pilkington.com))

## Teaching

2022 – Present:     Co-supervisor to 3 PhD students  
2019 – Present:     Proposed and supervised 7 final year Masters research projects at NTNU  
2021:                     Lecturer of Masters Course "TMT4245 FUNCTIONAL MATERIALS" at NTNU  
2014 – 2019:         Supervised 6 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)

## Computational Competence

UNIX/BASH/ZSH proficiency: high  
Python proficiency: high  
LaTEX proficiency: high  
VASP proficiency: high  
Adobe Creative Cloud proficiency: high

## Other Experience

2022 – Present:     Website, design, and general IT responsibility for the FACET group, NTNU

## References

|   |   |   |
|---|---|---|
| Prof. David O. Scanlon  | Prof. Tor Grande  | Prof. Sverre M. Selbach                                     |
| School of Chemistry   | Hovedbygningen, Gløshaugen                                | Department of Materials Science and Engineering             |
| University of Birmingham  | NTNU  | NTNU  |
| Birmingham  | Trondheim   | Trondheim   |
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