

Dr Benjamin A. D. Williamson

MSci MPhil PhD



Department of Materials Science and Engineering
Norwegian University of Science and Technology (NTNU)
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Nationality 🇬🇧 : British

🏢 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 – 1st Class Honours

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

Supervisor: Prof. David O. Scanlon

📖 Peer Reviewed Publications

(In reverse chronological order)

As of January 2025:

- Total Citations: 1416 (since 2017)

34. *Crystal Structure, Cation Occupation, and Phase Transitions in $Ba_4(Li_xNa_{1-x})_2Nb_{10}O_{30}$ Tetragonal Tungsten Bronzes*

N. S. Løndal, **B.A.D. Williamson**, O.G. Grendal, J. Walker, M.-E. Einarsrud, and T. Grande, *Inorganic Chemistry*, Advance Article, (2024)

DOI: 10.1021/acs.inorgchem.4c04461

33. *Mobile Intrinsic Point Defects for Conductive Neutral Domain Walls in LiNbO₃*
K. Eggestad, **B.A.D. Williamson**, D. Meier, and S. M. Selbach, *J. Mater. Chem. C*, 12, 17099-17107, (2024)
DOI: 10.1039/D4TC02856B
32. *Doping Implications of Li-ion Solid State Electrolyte Li₇La₃Zr₂O₁₂*
K. Eggestad, S. M. Selbach, and **B.A.D. Williamson**, *J. Mater. Chem. A*, 12, 15666-15675, (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 Ba₄M₂Nb₁₀O₃₀ (M = Na, K or Rb) and Ba₄M₂Nb₈Ti₂O₃₀ (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-RMnO₃ (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 TiO₂-Induced Current–Voltage Distortion in Sb₂Se₃ 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. Rignanese, S. Dwaraknath, J. Varley, K. A. Persson, M. Asta, G. Hautier; *npj Comp. Mater.*, 9, 1, 72 (2023)
DOI: 10.17188/mpcontribs/1907859
26. *Tuning the Thermoelectric Performance of CaMnO₃-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 ZnSb₂O₆*
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/acsenergylett.2c01961
24. *Mesophase transition in [(C₂H₅)N][FeBrCl₃] and [(CH₃)₄N][FeBrCl₃] 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 Ba₃Sc₂O₅Cu₂Se₂, Ba₃Y₂O₅Cu₂S₂, Ba₃Sc₂O₅Ag₂Se₂ and Ba₃In₂O₅Ag₂Se₂*
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 SnO₂*
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. *BaBi₂O₆: A Promising n-Type Thermoelectric Oxide with the PbSb₂O₆ 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>, 33, 7441, (2021)
DOI: 10.1021/acs.chemmater.1c02164
20. *Experimental and theoretical study of the electronic structures of lanthanide indium perovskites LnInO₃*
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 Ba₃Sc_{2-x}In_xCu₂S₂ and Ba₃In₂O₅Cu₂S_{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
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 Holy Grail of Transparent Electronics
DOI: 10.1016/j.matt.2020.08.008
17. *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
16. *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
15. *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
14. *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
13. *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
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 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

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. Instr.*, 89 (7), 073105 (2018)
DOI: 10.1063/1.5039829
8. *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
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 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
5. *Chemical Vapor Deposition Synthesis and Optical Properties of Nb₂O₅ 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 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
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

4. *Defect Chemistry and Kinetics of the Earth Abundant Li-Solid Electrolyte, X_xY_y*
B.A.D. Williamson, J.V. Renman, D. Rettenwander, A.M. Svensson, S.M. Selbach in submission
3. *Phase evolution and thermodynamics of cubic AX studied by high-temperature X-ray diffraction*
Ø. Gullbrekken, K. Eggestad, M. Tsoutsouva, **B.A.D. Williamson**, D. Rettenwander, M.-A. Einarsrud, S. Selbach, in submission

2. *Resonant XX Doping for High-Mobility In₂O₃-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. **Invited:** B.A.D Williamson: *Understanding CO₂ Transport using ARCS: Automated Reactions for CO₂ Storage*, MATHIAS Days conference, Total Energies, Paris, France 2024 – Talk
2. **Contributed:** B.A.D Williamson: *Computational Analysis of a Promising Earth Abundant, Stable, Lithium Solid Electrolyte.*, MRS Spring, Seattle, USA 2024 – Talk
3. **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
4. **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
5. **Contributed:** B.A.D. Williamson *Can we Utilise Phonons to Enhance Li-ion Diffusion?*, MRS Fall Meeting, Boston, USA 2022 –Talk
6. **Contributed:** B.A.D. Williamson *The Underlying Mechanisms of Ultrahigh Mobility in Bi₂O₂Se using Self-Consistent GW Method*, MRS Spring Meeting, Honolulu, USA 2022 –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 discovery of an earth abundant, stable Li solid electrolyte*, FACET Sustainability Workshop, Trondheim, Norway 2021 –Talk
9. **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
10. **Contributed:** B.A.D Williamson: *Resonant Doping for High Mobility Transparent Conductors: The Case of Mo-doped In₂O₃*, 11th Petite Workshop on defects in energy materials; Sommarøy, Norway 2019 – Talk
11. **Contributed:** B.A.D Williamson: *Computationally Aided Discovery of Layered Quinary Oxychalcogenide p-type Transparent Conductor*, Workshop For Atomistic Modelling; Trondheim, Norway 2019 – Poster
12. **Contributed:** B.A.D Williamson: *Dispelling the Myth of Passivated Codoping in TiO₂*, MRS Fall Meeting; Boston US, 2018 – Talk
13. **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
14. **Contributed:** B.A.D Williamson: *Doubled Conductivity in Transparent Conducting In₂O₃ Through Novel Dopant Design*, MMM Hub; Thomas Young Centre, London, UK, 2018 – Poster
15. **Invited:** B.A.D Williamson: *Doubled Conductivity in Transparent Conducting In₂O₃ Through Novel Dopant Design*, MCC 3rd Conference, Lincoln UK, 2018 – Talk
16. **Contributed:** B.A.D Williamson: *Doubled Conductivity in Transparent Conducting In₂O₃ Through Novel Dopant Design*, Gordon Research Conference; Defects In Semiconductors, Colby-Sawyer College, New Hampshire, US, 2018 – Poster
17. **Invited:** B.A.D Williamson: *Beyond Conventional Doping in SnO₂*, Thomas Young Centre, London UK, 2017 – Talk
18. **Contributed:** B.A.D Williamson: *Beyond Conventional Doping in SnO₂*, E-MRS; Spring Meeting, Strasbourg France, 2017 – Poster

19. **Contributed:** B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, E-MRS; Spring Meeting, Strasbourg France, 2017 – Talk
20. **Contributed:** B.A.D Williamson: *Engineering Valence Band Dispersion For High-Mobility p-type Semiconductors*, MRS Fall Meeting; Boston US, 2016 – Poster
21. **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)
 2021 – Present: Equinor (www.equinor.com)
 Northern Lights (www.northernlightsccs.com)
 Total Energies (www.totalenergies.com)
 Shell (www.shell.com)
 2014 – 2019: Pilkingtons NSG Group (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 1st year workshops (CHEM1004)
 2018 – 2019: Tutor in 1st year inorganic chemistry courses at UCL (CHEM1101 and CHEM0013)

Computational Competance

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
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