Dr Benjamin A. D. Williamson MSci MPhil PhD



Department of Materials Science and Engineering Norwegian University of Science and Technology (NTNU) 7491 Trondheim Norway

Email : benjamin.williamson@ntnu.no

Website/Github 🖸 : badw.github.io

Google Scholar G: scholar.google.com/citations?user=c34AgtMAAAAJ

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Nationality : British

L 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 April 2025:

- Total Citations: 1474

37. Quantifying Emptiness: On the Size of A-Site Vacancies in Tetragonal Tungsten Bronzes

C. R. Zeiger, K. Eggestad, J. Walker, M.-A. Einarsrud, B.A.D. Williamson, and T. Grande Chemistry of

Materials, ASAP, (2025)

DOI: 10.1021/acs.chemmater.4c03438

36. Phase Evolution and Thermodynamics of Cubic $Li_{6.25}Al_{0.25}La_3Zr_2O_{12}$ Studied by High-Temperature X-ray Diffraction

Ø. Gullbrekken, K. Eggestad, M. Tsoutsouva, **B.A.D. Williamson**, D. Rettenwander, M.-A. Einarsrud, and S. M. Selbach *Inorganic Chemistry*, 64, 12, 5866-5865, (2025)

DOI: 10.1021/acs.inorgchem.4c03738

35. Pseudo-Lithium Vacancies in Hydrogen Rich Li₃OCl

B.A.D. Williamson, K. Eggestad, S. M. Selbach *J. Mater. Chem. A*, 13, 8816-8824, (2025) DOI: 10.1039/D4TA08352K

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 $Ba_4M_2Nb_{10}O_{30}$ (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-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. Willamson**, 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 Gadoped ZnSb₂O₆

A. J. Jackson, B. J. Parrett, J. Willis, A. M. Ganose, W. W. W. Leung, **B.A.D. Willamson**, 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. Willamson**, 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 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.0c11592pted, 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 $Ba_3Sc_{2-x}In_xCu_2S_2$ 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

18. 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

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 ${\it TiO}_2$ 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

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 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

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. Inst.*, 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 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

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

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. Defect Chemistry and Kinetics of the Earth Abundant Li-Solid Electrolyte, X_xY_y **B.A.D. Willamson**, J.V Renman, D. Rettenwander, A.M. Svensson, S.M. 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

Conference Presentations

- 1. *Invited*: B.A.D Williamson: *Understanding CO*₂ *Transport using ARCS*: *Automated Reactions for CO*₂ *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 Bi*₂O₂Se 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 In_2O_3 , 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 TiO*₂, 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 In*₂O₃ *Through Novel Dopant Design*, MCC 3rd Conference, Lincoln UK, 2018 Talk

- 16. Contributed: B.A.D Williamson: *Doubled Conductivity in Transparent Conducting In*₂O₃ *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 SnO*₂, Thomas Young Centre, London UK, 2017 Talk
- 18. Contributed: B.A.D Williamson: *Beyond Conventional Doping in SnO*₂, 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

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