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
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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

As of October 2024:

Total Citations: 1330 (since 2017)

h-index: 19

(In reverse chronological order)

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, Advance Article, (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 $Ba_4M_2Nb_{10}O_{30}$ $(M = Na, K \text{ or } Rb) \text{ and } Ba_4M_2Nb_8Ti_2O_{30} \text{ } (M = Ca \text{ or } Sr)$

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 microstructur-

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 $[(C_2H_5)N]$ [FeBrCl₃] and $[(CH_3)_4N]$ [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 Ba₃Sc₂O₅Cu₂Se₂, Ba₃Y₂O₅Cu₂S₂, Ba₃Sc₂O₅Ag₂Se₂ 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 $Ba_3In_2O_5Cu_2S_{2-v}Se_v$

G. Limburn, M. Štephens, **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 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 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

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. Willamson**, 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 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*₂O₃, 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_2O_3 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
- 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 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

k→ References

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