# Dr Benjamin A. D. Williamson

# MSci, PhD

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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
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$^{st}$ Class Honours
MSci dissertation title: *Computational Design of Next-Generation p-Type Semiconductors*
Supervisor: Prof. David O. Scanlon

## Publications

As of July 2024:
Total Citations: 1252
*h*-index: 18
(In reverse chronological order)

1. *Doping Implications of Li-ion Solid State Electrolyte $Li_7La_3Zr_2O_{12}$*
K. Eggestad, 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

2. *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

3. *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

4. *Oxygen absorption in nanocrystalline h-$RMnO_3$ (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

5. *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

6. *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

7. *Tuning the Thermoelectric Performance of $CaMnO_3$-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

8. *Computational Prediction and Experimental Realisation of Earth Abundant Transparent Conducting Oxide Ga-doped $ZnSb_2O_6$*
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

9. *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. 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

10. *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

11. *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

12. *$BaBi_2O_6$: 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.0c11592pted*, 33, 7441, (2021)
DOI: 10.1021/acs.chemmater.1c02164

13. *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*, 125, 6387, (2021)
DOI: 10.1021/acs.jpcc.0c11592

14. *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

15. *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

16. *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

17. *Resonant Ta Doping for Enhanced Mobility in Transparent Conducting $SnO_2$*
**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

18. *Enhanced Photocatalytic and Antibacterial Ability of Cu-doped Anatase $TiO_2$ 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

19. *Resonant Doping for High Mobility Transparent Conductors: The Case of Mo-doped $In_2O_3$*
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

20. *Dispelling the Myth of Passivated Codoping in $TiO_2$*
**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

21. *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

22. *Phosphorus Doped $SnO_2$ 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

23. *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

24. *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

25. *Chemical Vapor Deposition of Photocatalytically Active Pure Brookite $TiO_2$ 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

26. *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

27. *Self-Compensation in Transparent Conducting F-Doped $SnO_2$*
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

28. *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

29. *Computational and Experimental Study of $Ta_2O_5$ 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

30. *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

31. *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

32. *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*

1. *Mobile Point Defects for Conductive and Memristive Domain Walls in $ABO_3$*
K. Eggestad, **B.A.D. Williamson**, and S. M. Selbach, *in submission*

2. *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*

3. *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 $Bi_2O_2Se$ 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 $In_2O_3$*, 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 $TiO_2$*, 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 $In_2O_3$ Through Novel Dopant Design*, MMM Hub; Thomas Young Centre, London, UK, 2018 – Poster
14. *Invited:* B.A.D Williamson: *Doubled Conductivity in Transparent Conducting $In_2O_3$ Through Novel Dopant Design*, MCC 3rd Conference, Lincoln UK, 2018 – Talk
15. 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
16. *Invited:* B.A.D Williamson: *Beyond Conventional Doping in $SnO_2$*, Thomas Young Centre, London UK, 2017 – Talk
17. Contributed: B.A.D Williamson: *Beyond Conventional Doping in $SnO_2$*, 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

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|---|---|
| 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

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| 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$^{st}$ year workshops (CHEM1004) |
| 2018 – 2019: | Tutor in 1$^{st}$ 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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