

National University of Singapore
Materials Science and Engineering
9 Engineering Drive 1
Singapore, 117576

Office: Block EA, #02-03
ORCID: orcid.org/0000-0002-5168-9253
Email: pcanepa@nus.edu.sg
URL: caneparesearch.org

Appointments

2018–present Assistant Professor, Materials Science and Engineering, NUS
2018–present Joint Assistant Professor, Chemical and Biomolecular Engineering, NUS
2018–present Investigator in the Singapore-MIT Alliance

Professional Preparation & Education

2017–2018	University of Bath (UK)	Independent Ramsay Memorial Fellow
2013–2017	Massachusetts Institute of Technology (USA) Lawrence Berkeley National Laboratory (USA) Advisor: Prof. Gerbrand Ceder	PostDoctoral Fellow
2011–2013	Wake Forest University (USA) Advisor: Prof. Timo Thonhauser	PreDoctoral + PostDoctoral Fellow
2009–2012	University of Kent (UK) Advisors: Prof.s M. Aldfredsson & A. Chadwick	Ph.D., Chemistry
2006–2008	University of Turin (Italy)	M.Sc., Chemistry
2003–2006	University of Turin (Italy)	B.Sc., Chemistry

Honours & Awards

August 2021 Fellow of the Royal Society of Chemistry, London (UK)
March 2021 EU ERC MSEC+ Erasmus mundus Scholar, 2021, France
<https://mesc-plus.eu/application/scholar>
March 2020 Singapore NRF Fellow Class 2020
May 2017 Royal Society of Chemistry Travel Grant for Early Career Scientists
November 2016 Ramsay Memorial Fellow, University College London, London (UK)
April 2015 US Department of Energy, Advanced Scientific Computing Leadership Challenge
August 2013 US National Science Foundation —Peer mentor award

Research Grants & Other Funding

At NUS

2020–2025	NRF Fellowship (success rate $\leq 5\%$), S\$2,787,033, PI, ID: NRFF12-2020-0012 <i>Designing Functional Interfaces of Batteries Using Theory and Computation</i>
2020–2023	ANR-NRF (success rate $\leq 5\%$), S\$449,999, PI, ID: NRF2019-NRF-ANR073 <i>Nanostructured Materials for Advanced Na SolidsTate battERies–Na-MASTER</i>
2020–2025	NRF Competitive Research Programme, S\$8,765,704, Co-PI, ID: NRF-CRP22-2019-0008 <i>Large Area Synthesis and Applications of Atomically Thin Amorphous Materials</i>
2021	Australian Centre for Neutron Scattering, AU\$181,610, PI, ID: 9697 <i>Unlocking the complex structure-property relationships in NaSICON electrolytes</i>
2020	Australian Centre for Neutron Scattering, AU\$34,200, PI, ID: 8303 <i>Structural studies of phases within the LiX to Li₃PS₄ family</i>
2018–2022	Start-up grant, Ministry of Education Tier-1, S\$250,000, PI, R-284-000-186-133 <i>Achieving High Energy-Density and Safety in Lithium-ion Batteries</i>
2018–2021	Ministry of Education Tier-1, S\$120,000, Role: PI, ID: R-284-000-194-114 <i>Functional Metal-Organic Framework Materials for Energy Applications</i>
2021	Dyson PTE LTD, S\$95,000.00, Role: PI
2018–2023	Co-PI, NUS Flagship Green Energy Program, NUS, Singapore
2019–present	Several multimillion CPU/hour grants from the National Supercomputing Centre Singapore

Before NUS

2016–2018	Ramsay Memorial Fellowship, University College London, Role: PI, £78,000
2017	Royal Society of Chemistry Travel Grant for Early Career Scientists
2015	US DOE, Advanced Scientific Computing Leadership 98,000,000 CPU/hours equipment grant-equivalent \$980,000 at \$0.01 per CPU/hour, Argonne, IL, USA.
2009–2012	PhD Scholarship, School of Physical Sciences, University of Kent, UK

Peer-reviewed Publications

Publications as Principal Investigator

†Publications as Corresponding Author

70. #Invited V. Kapoor, B. Singh, Z. Wang, G. Sai Gautam, A. K. Cheetham, and **P. Canepa**[†], *Rational Design of Mixed Polyanion Electrodes for Sodium-ion Batteries*, **Chem. Mater.** Special edition: “John Goodenough at 100” invited and to be submitted (IF: 10.1)
69. #Y. Li, A. M. Prabhu, T. S. Choksi and **P. Canepa**[†], *H₂O and CO₂ Surface Contamination of Li₇La₃Zr₂O₁₂ as a Case for Catalysis on Complex Oxides*, under revision in **J. Mater. Chem. A** (2021) (IF: 12.732) (2021).

68. #Z. Deng, T. P. Mishra, E. Mahayoni, J.-N. Chotard, V. Seznec, A. K. Cheetham, C. Masquelier, G. Sai Gautam, and **P. Canepa**[†], *Theoretical and Experimental Studies of ion Transport in Mixed Polyanion Solid Electrolytes*, under revision in **Nature Commun.** (2021). [10.21203/rs.3.rs-1102507/v1](https://doi.org/10.21203/rs.3.rs-1102507/v1)
67. #E. Sebt, H. A. Evans, H. Chen, P. M. Richardson, K. White, R. Giovine, E. Gonzalez-Correa, C. M. Brown, A. K. Cheetham, **P. Canepa**[†], R. J. Clément, *Stacking fault susceptibility of superionic conductor Li_3YCl_6* , (2021) under revision in **J. Amer. Chem. Soc.**
66. T. P. Mishra, C. Li, S. Gradečak, **P. Canepa**, and S. J. Pennycook, *Channeling-enhanced depth resolution in scanning transmission electron microscopy*, (2021) under revision
65. L. Tao, S. Saqlinea, Q. Fan, Z. Deng, M. Dunstan, Y. Dai, **P. Canepa**, and P. Liu, *Large scale computational and experimental screening of novel materials as oxygen carriers for chemical looping dry reforming of methane*, (2021) under revision in **Adv. Func. Materials**
64. #H. A. Evans, D. Mullangi, Z. Deng, Y. Wang, S. B. Peh, F. Wei, J. Wang, C. M. Brown, D. Zhao, **P. Canepa**[†], A. K. Cheetham, *Highly selective CO_2 capture from wet flue gas with the metal-organic framework aluminum formate*, (2021) under 2nd revision in **Science**.
63. #Invited Y. Gao, T. P. Mishra, S.-H. Bo, G. Sai Gautam and **P. Canepa**[†], *Design and Characterization of Host-Frameworks for Facile Magnesium Transport*, **Annu. Rev. Mater. Res.** (2022) accepted and in press (IF: 16.286)
62. #Invited Editorial M. M. Doeff, R. J. Clément, and **P. Canepa**[†], *Solid Electrolytes in the Spotlight*, **Chem. Mater.**, (2022) [10.1021/acs.chemmater.1c03770](https://doi.org/10.1021/acs.chemmater.1c03770). (IF: 10.1)
61. #S. Park, Z. Wang, Z. Deng, D. Carlier, I. Moog, F. Fauth, **P. Canepa**[†], L. Croguennec, C. Masquelier, and J.-N. Chotard, *Crystal Structure of $\text{Na}_2\text{V}_2(\text{PO}_4)_3$, an Intriguing Phase Spotted in the $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ - $\text{NaV}_2(\text{PO}_4)_3$ system* (2021) accepted in **Chem. Mater.** (IF: 10.1)
60. #Invited Z. Deng, V. Kumar, F. T. Bölle, F. Caro, A. A. Franco, I. E. Castelli, **P. Canepa**[†], and Zhi Wei Seh, *Towards Autonomous High-Throughput Multiscale Modelling of Battery Interfaces*, (2021) accepted in **Energy Environ. Sci.** (IF: 38.532)
59. #Z. Wang, S. Park, Z. Deng, D. Carlier, J.-N. Chotard, L. Croguennec, G. Sai Gautam, A. K. Cheetham, C. Masquelier and **P. Canepa**[†], *Phase Stability and Sodium-Vacancy Orderings in a NaSICON electrode*, (2021) **J. Mater. Chem. A** (2021) (IF: 12.732) [10.1039/D1TA09249A](https://doi.org/10.1039/D1TA09249A). (IF: 12.732)
Selected by the J. Mater. Chem. A as HOT Papers
58. #P. Gorai, B. Singh, V. Stevanović and **P. Canepa**[†], *Devil is in the Defects: Electronic Conductivity in Solid Electrolytes*, **Chem. Mater.**, 33, 18, 7484 (2021) [10.1021/acs.chemmater.1c02345](https://doi.org/10.1021/acs.chemmater.1c02345). (IF: 10.1)

57. #W. Lu, J. Wang, G. S. Gautam **P. Canepa**[†], *Searching Ternary Oxides and Chalcogenides as Positive Electrodes for Calcium Batteries*, **Chem. Mater.**, 33, 14, 5809 (2021) [10.1021/acs.chemmater.1c01992](https://doi.org/10.1021/acs.chemmater.1c01992). (IF: 10.1)
56. #C. Hänsel, B. Singh, **P. Canepa**[†] and D. Kundu, *Favorable Interfacial Chemomechanics Enables Stable Cycling of High Li-Content Li–In/Sn Anodes in Sulfide Electrolyte Based Solid-State Batteries*, **Chem. Mater.**, 33, 15, 6029 (2021) [10.1021/acs.chemmater.1c01431](https://doi.org/10.1021/acs.chemmater.1c01431). (IF: 10.1)
55. T. Famprikis, H. Bouyanfif, **P. Canepa**, M. Zbiri, J. Dawson, E. Suard, F. Fauth, H. Y. Playford, D. Dambournet, O. J. Borkiewicz, M. Courty, O. Clemens, J.-N. Chotard, S. Islam, C. Masquelier, *Insights into the rich polymorphism of the Na⁺ ion conductor Na₃PS₄ from the perspective of variable-temperature diffraction and spectroscopy*, **Chem. Mater.**, 33, 5652 (2021) [10.1021/acs.chemmater.1c01113](https://doi.org/10.1021/acs.chemmater.1c01113). (IF: 10.1)
54. #T. P. Mishra, G. J. Syaranamual, Z. Deng, J.-Y. Chung, L. Zhang, S. A. Goodman, L. Jones, M. Bosman, S. Gradečak, S. J. Pennycook, and **P. Canepa**[†], *Unlocking the origin of compositional fluctuations in InGaN light emitting diodes*, **Phys. Rev. Mater.**, 00, 004600 (2021). [10.1103/PhysRevMaterials.00.004600](https://doi.org/10.1103/PhysRevMaterials.00.004600). (IF: 3.989)
53. #A. Symington, M. Molinari, J. A. Dawson, J. Statham, J. Purton, **P. Canepa**[†] and S. Parker, *Elucidating the Nature of Grain Boundary Resistance in Lithium Lanthanum Titanate*, **J. Mater. Chem. A**, 9, 6487 (2021) [10.1039/D0TA11539H](https://doi.org/10.1039/D0TA11539H). (IF: 12.732)
52. #B. Singh, Z. Wang, S. Park, G. S. Gautam, J.-N. Chotard, L. Croguennec, D. Carlier, A. K. Cheetham, C. Masquelier and **P. Canepa**[†], *A Chemical Map of NaSiCON Electrode Materials for Sodium-ion Batteries*, **J. Mater. Chem. A**, 9, 281 (2021) [10.1039/D0TA10688G](https://doi.org/10.1039/D0TA10688G). (IF: 12.732)
Selected by the J. Mater. Chem. A as HOT Papers
51. T. Famprikis, O. U. Kudu, J. Dawson, **P. Canepa**, F. Fauth, E. Suard, M. Zbiri, D. Dambournet, O. Borkiewicz, H. Bouyanfif, S. Emge, C. P. Grey, S. Cretu, J.-N. Chotard, W. Zeier, S. Islam, C. Masquelier, *Under Pressure: Mechanochemical Effects on Structure and Ion Conduction in the Sodium-Ion Solid Electrolyte Na₃PS₄*, **J. Am. Chem. Soc.**, 142, 1842 (2020) [10.1021/jacs.0c06668](https://doi.org/10.1021/jacs.0c06668). (IF: 15.419)
50. #Z. Deng, S. G. Gopalakrishnan, S. K. Kolli, J.-N. Chotard, A. K. Cheetham, C. Masquelier and **P. Canepa**[†], *Phase Behavior in Rhombohedral NaSiCON Electrolytes and Electrodes*, **Chem. Mater.**, 32, 7908 (2020) [10.1021/acs.chemmater.0c02695](https://doi.org/10.1021/acs.chemmater.0c02695). (IF: 10.1).
49. #J. Forero-Saboya, C. Davoisne, R. Dedryvere, I. Yousef, A. Ponrouch, **P. Canepa**[†] *Understanding the nature of the passivation layer on calcium electrodes in calcium batteries*, **Energy Environ. Sci.**, 13, 3423 (2020) [10.1039/D0EE02347G](https://doi.org/10.1039/D0EE02347G). (IF: 38.532)
48. #Z. Deng, F. Wei, Y. Wu, R. Seshadri, A. K. Cheetham, and **P. Canepa**[†] *Understanding the Structural and Electronic Properties of Bismuth Trihalides and Related Compounds*, **Inorg. Chem.**,

- 59, 6, 3377-3386 (2020) [10.1021/acs.inorgchem.9b03214](https://doi.org/10.1021/acs.inorgchem.9b03214). (IF: 4.85)
47. T. Famprikis, **P. Canepa**, J. Dawson, M. S. Islam and C. Masquelier, *Fundamentals of Inorganic Solid State Electrolytes for Batteries*, **Nature Materials** 18, 1278 (2019). [10.1038/s41563-019-0431-3](https://doi.org/10.1038/s41563-019-0431-3). (IF: 48.386)
46. #T. Chen, S. G. Gopalakrishnan and **P. Canepa**[†], *Ionic Transport in Potential Coating Materials for Mg Batteries*, **Chem. Mater.** 31 (19), 8087 (2019). [10.1021/acs.chemmater.9b02692](https://doi.org/10.1021/acs.chemmater.9b02692). (IF: 10.1)
45. #T. W. Kasel, Z. Deng, A. M. Mroz, C. H. Hendon, K. Butler, **P. Canepa**[†], *Metal-free perovskites for non-linear optical materials*, **Chem. Sci.** 10, 8187 (2019), [10.1039/C9SC03378E](https://doi.org/10.1039/C9SC03378E). (IF: 10.0)
44. #Invited S. G. Gopalakrishnan and **P. Canepa**[†], *Theoretical modelling of multivalent ions in inorganic hosts*. Chapter 4, 79–113 (2020). This chapter is part of the book with title *Magnesium Batteries* edited by M. Fichtner; Series: Energy and Environment Series RSC. [10.1039/9781788016407-00079](https://doi.org/10.1039/9781788016407-00079).
43. J. Dawson, **P. Canepa**, M. J. Clarke, T. Famprikis, D. Ghosh and M. S. Islam, *Towards Understanding the Different Influences of Grain Boundaries on Ion Transport in Sulfide and Oxide Solid Electrolytes*, **Chem. Mater.** 31 (14), 5296 (2019). [10.1021/acs.chemmater.9b01794](https://doi.org/10.1021/acs.chemmater.9b01794). (IF: 10.1)
42. #Invited K. T. Butler, S. G. Gopalakrishnan and **P. Canepa**[†], *Designing interfaces in energy materials applications with first-principles calculations*, **npj Comput. Mater.** 19 (2019) [10.1038/s41524-019-0160-9](https://doi.org/10.1038/s41524-019-0160-9). (IF: 13.993)
41. #T. Chen, G. Ceder, Gopalakrishnan and **P. Canepa**[†], *Evaluation of Mg compounds as coating materials in Mg batteries*, **Front. Chem.** 8, 1759 (2019). [10.3389/fchem.2019.00024](https://doi.org/10.3389/fchem.2019.00024). (IF: 4.155)
40. #F. Meutzner, T. Nestler, M. Zschornak, **P. Canepa**, S. G. Gopalakrishnan, S. Leoni, S. Adams, T. Leisegang, V. A. Blatov and D. C. Meyer, *Computational analysis and identification of battery materials*, **Phys. Sci. Rev.** (2018). [10.1515/psr-2018-0044](https://doi.org/10.1515/psr-2018-0044). (IF: NA)
39. J. A. Dawson, **P. Canepa**, T. Famprikis, C. Masquelier and M. S. Islam, *Correction to Atomic-Scale Influence of Grain Boundaries on Li-Ion Conduction in Solid Electrolytes for All-Solid-State Batteries*, **J. Am. Chem. Soc.** 140, 7044 (2018) [10.1021/jacs.8b04915](https://doi.org/10.1021/jacs.8b04915). (IF: 15.419)
38. J. A. Dawson, **P. Canepa**, T. Famprikis, C. Masquelier and M. S. Islam, *Atomic-Scale Influence of Grain Boundaries on Li-ion Conduction in Solid Electrolytes for All-Solid-State Batteries*, **J. Am. Chem. Soc.** 140, 362 (2018) [10.1021/jacs.7b10593](https://doi.org/10.1021/jacs.7b10593). (IF: 15.419)
37. **P. Canepa**[†], J. A. Dawson, S. G. Gopalakrishnan, J. M. Statham, S. C. Parker, and M. S. Islam, *Particle Morphology and Lithium Segregation to Surfaces of the $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Solid Electrolyte*, **Chem. Mater.** 30, 3019 (2018). [10.1021/acs.chemmater.8b00649](https://doi.org/10.1021/acs.chemmater.8b00649). (IF: 10.1)

Publications as a PostDoctoral fellow & PhD Student

36. R. Bayliss, B. Key, S. G. Gopalakrishnan, **P. Canepa**, B. Jin Kwon, S. Lapidus, F. Dogan, A. Adil, A. Lipton, P. Baker, G. Ceder, J. Vaughey and J. Cabana *Probing Mg Migration in Spinel Oxides*, **Chem. Mater.** 32, 663 (2020). [10.1021/acs.chemmater.9b02450](https://doi.org/10.1021/acs.chemmater.9b02450). (IF: 10.1)
35. **P. Canepa**[†], S.-H. Bo, S. G. Gopalakrishnan, W. D. Richards, Y. Wang, S. G. Gopalakrishnan and G. Ceder, *High Magnesium Mobility in Ternary Spinel Chalcogenides*, **Nature Commun.** 8, 1759 (2017). [10.1038/s41467-017-01772-1](https://doi.org/10.1038/s41467-017-01772-1). (IF: 13.610)
34. D. C. Hannah, S. G. Gopalakrishnan, **P. Canepa** and G. Ceder, *On the Balance of Intercalation and Conversion Reactions in Battery Cathodes*, **Adv. Energy Mater.** 8, 1800379 (2018). [10.1002/aenm.201800379](https://doi.org/10.1002/aenm.201800379). (IF: 25.245)
33. **P. Canepa**[†], S. G. Gopalakrishnan, D. Broberg, S.-H. Bo and G. Ceder, *The role of point defects in Mg chalcogenide spinel conductors*, **Chem. Mater.** 29, 9657 (2017). [10.1021/acs.chemmater.7b02909](https://doi.org/10.1021/acs.chemmater.7b02909). (IF: 10.1)
32. [†]S. G. Gopalakrishnan,* **P. Canepa**,* S.-H. Bo and G. Ceder, *Influence of inversion on Mg mobility in spinels*, **Chem. Mater.** 29, 7918 (2017) [10.1021/acs.chemmater.7b02820](https://doi.org/10.1021/acs.chemmater.7b02820). (IF: 10.1) *co-first author
31. **P. Canepa**[†], S. G. Gopalakrishnan, D. C. Hannah, R. Malik, M. Liu, K. Gallagher, K. Persson and G. Ceder, *Odyssey of Multivalent Cathode Materials: Open Questions and Future Challenges*, **Chem. Rev.** 117, 4287 (2017) [10.1021/acs.chemrev.6b00614](https://doi.org/10.1021/acs.chemrev.6b00614). (IF: 60.622)
30. D. C. Hannah, S. G. Gopalakrishnan, **P. Canepa**, Z. Rong and G. Ceder, *Magnesium Ion Mobility in Post-Spinels Accessible at Ambient Pressure*, **Chem. Comm.** 53, 5171 (2017) [10.1039/C7CC01092C](https://doi.org/10.1039/C7CC01092C). (IF: 6.222)
29. M. Liu, A. Jain, X. Qu, Z. Rong, **P. Canepa**, R. Malik, G. Ceder and K. Persson, *Evaluation of sulfur spinel compounds for multivalent battery cathode applications*, **Energy Environ. Sci.** 9, 3201 (2016) [10.1039/C6EE01731B](https://doi.org/10.1039/C6EE01731B). (IF: 38.532)
28. K. Tan, S. Zuluaga, H. Wang, **P. Canepa**, K. Soliman, J. Li, T. Thonhauser, and Y. J. Chabal, *Interaction of acid gases SO₂, NO₂ with Coordinatively Unsaturated Metal Organic Frameworks: M-MOF-74 (M= Zn, Mg, Ni, Co)*, **Chem. Mater.** 29, 4227 (2017) [10.1021/acs.chemmater.7b00005](https://doi.org/10.1021/acs.chemmater.7b00005). (IF: 10.1)
27. Y. Ihm, V. R. Cooper, L. Vlcek, **P. Canepa**, T. Thonhauser, J. H. Shim, and J. R. Morris, *CMGIF: predictive Continuum Model of Gas uptake for Inhomogeneous Fluids*, accepted in **J. Phys. Chem. C** 121, 17625 (2017). [10.1021/acs.jpcc.7b04834](https://doi.org/10.1021/acs.jpcc.7b04834). (IF: 4.126)
26. Z. Rong, D. Kitchaev, **P. Canepa**, W. Huang and G. Ceder, *An efficient algorithm for finding the minimum energy migration path in ionic materials*, **J. Chem. Phys.** 145, 074112 (2016)

[10.1063/1.4960790](#). (IF: 3.488)

25. S. Berto, E. Chiavazza, **P. Canepa**, E. Prenesti and P. G. Daniele, *Assessing the formation of weak sodium complexes with negatively charged ligands*, **Phys. Chem. Chem. Phys.** 18, 13118 (2016) [10.1039/C6CP00192K](#). (IF: 4.123)
24. S. G. Gopalakrishnan, **P. Canepa**, W. D. Richards, R. Malik and G. Ceder, *Role of structural H₂O in intercalation electrodes: the case of Mg in Nanocrystalline Xerogel-V₂O₅*, **Nano. Lett.** 16, 2426 (2016) [10.1021/acs.nanolett.5b05273](#). (IF: 11.189)
23. **P. Canepa**[†], S. Jayaraman, L. Cheng, N. N. Rajput, S. G. Gopalakrishnan, L. A. Curtis, K. A. Persson and G. Ceder, *Elucidating the structure of the magnesium aluminum chloride complex electrolyte for magnesium-ion batteries*, **Energy Environ. Sci.** 8, 3718 (2015) [10.1039/C5EE02340H](#). (IF: 38.532)
22. S. G. Gopalakrishnan, **P. Canepa**, R. Malik, M. Liu, K. Persson and G. Ceder, *First-principles evaluation of Multi-Valent cation insertion into Orthorhombic V₂O₅*, **Chem. Comm.** 51, 13619 (2015) [10.1039/C5CC04947D](#). (IF: 6.222)
21. Z. Rong, R. Malik, **P. Canepa**, S. G. Gopalakrishnan, M. Liu, A. Jain, K. Persson and G. Ceder, *Materials Design Rules for Multi-Valent Ion Mobility in Intercalation Structures*, **Chem. Mater.** 27, 6016 (2015) [10.1021/acs.chemmater.5b02342](#). (IF: 10.1)
20. S. G. Gopalakrishnan, **P. Canepa**, A. Abdellahi, A. Urban, R. Malik and G. Ceder, *The Intercalation phase diagram of Mg in V₂O₅ from first-principles*, **Chem. Mater.** 27, 3733 (2015) [10.1021/acs.chemmater.5b00957](#). (IF: 10.1)
19. **P. Canepa**[†], S. G. Gopalakrishnan, R. Malik, S. Jayaraman, Z. Rong, K. R. Zavadil, K. A. Persson and G. Ceder, *Understanding the Initial Stages of Reversible Mg Deposition and Stripping in Inorganic Non-Aqueous Electrolytes*, **Chem. Mater.** 27, 3317 (2015) [10.1021/acs.chemmater.5b00389](#). (IF: 10.1)
18. M. Liu, Z. Rong, R. Malik, **P. Canepa**, A. Jain, G. Ceder and K. A. Persson, *Spinel Compounds as Multivalent Battery Cathodes: A Systematic Evaluation Based on ab initio Calculations*, **Energy Environ. Sci.** 8, 964 (2015) [10.1039/C4EE03389B](#). (IF: 38.532)
17. **P. Canepa**, K. Tan, Y. Du, H. Lu, Y. J. Chabal and T. Thonhauser, *Structural, elastic, thermal, and electronic response of small-molecule- loaded metal organic framework materials*, **J. Mater. Chem. A** 3, 986 (2015). [10.1039/C4TA03968H](#). (IF: 12.732)
Journal cover **J. Mater. Chem. A** 3, 919 (2015) [10.1039/C5TA90011E](#).
16. K. Tan, S. Zuluaga, Q. Gong, **P. Canepa**, J. Li, T. Thonhauser, and Y. J. Chabal, *Water Reaction Mechanism in Metal Organic Frameworks with Coordinatively Unsaturated Metal Ions: (MOF-74)*, **Chem. Mater.** 26, 6886 (2014) [10.1021/cm5038183](#). (IF: 10.1)

15. S. Zuluaga Botero, **P. Canepa**, K. Tan, T. Thonhauser and Y. J. Chabal, *Study of van der Waals bonding and interactions in metal organic framework materials*, **J. Phys.: Condens. Matter.** 26, 133002 (2014) [10.1088/0953-8984/26/13/133002](https://doi.org/10.1088/0953-8984/26/13/133002). (IF: 2.333)
14. K. Tan, **P. Canepa**, Q. Gong, J. Liu, D. H. Johnson, P. Thallapally, T. Thonhauser, J. Li and Y. J. Chabal, *Mechanism of preferential adsorption of SO₂ into two microporous paddle wheel frameworks M(bdc)(ted)_{0.5}*, **Chem. Mater.** 25, 4653 (2013) [10.1021/cm401270b](https://doi.org/10.1021/cm401270b). (IF: 10.1)
13. **P. Canepa**, C. A. Alter, E. M. Conwill, D. H. Johnson, B. A. Shoemaker, K. Z. Soliman and T. Thonhauser, *High-throughput screening of small-molecule adsorption in MOF*, **J. Mater. Chem. A** 1 (43), 13597 (2013) [10.1039/C3TA12395B](https://doi.org/10.1039/C3TA12395B). (IF: 12.732)
12. N. Nijem, **P. Canepa**, U. Kaipa, K. Tan, K., et al., *Water cluster confinement and methane adsorption in the hydrophobic cavities of a fluorinated metal-organic framework*, **J. Am. Chem. Soc.** 135, 12615 (2013) [10.1021/ja400754p](https://doi.org/10.1021/ja400754p). (IF: 15.419)
11. M. G. Lopez, **P. Canepa** and T. Thonhauser, *Using NMR to study small molecule adsorption in MOF-74-Mg*, **J. Chem. Phys.** 138, 154704 (2013) [10.1063/1.4800952](https://doi.org/10.1063/1.4800952). (IF: 3.488)
10. **P. Canepa**, Y. J. Chabal and T. Thonhauser, *When Metal Organic Frameworks turn into Linear Magnets*, **Phys. Rev. B** 87, 094407 (2013) [10.1103/PhysRevB.87.094407](https://doi.org/10.1103/PhysRevB.87.094407). (IF: 4.036)
9. **P. Canepa**, N. Nijem, Y. J. Chabal and T. Thonhauser, *Diffusion of Small Molecules in Metal Organic Framework Materials*, **Phys. Rev. Lett.** 110, 026102 (2013) [10.1103/PhysRevLett.110.026102](https://doi.org/10.1103/PhysRevLett.110.026102). (IF: 9.161)
8. N. Nijem, **P. Canepa**, H. Wu, A. Marti, K. Balkus Jr., T. Thonhauser, J. Li and Y. J. Chabal, *Tuning the Gate Opening Pressure of MOFs for the Selective Adsorption of Hydrocarbons*, **J. Am. Chem. Soc.** 134, 15201 (2012) [10.1021/ja305754f](https://doi.org/10.1021/ja305754f). (IF: 15.419)
7. K. Tan, N. Nijem, **P. Canepa**, Q. Gong, J. Li, T. Thonhauser, and Y. J. Chabal, *Stability and Hydrolyzation of Metal Organic Frameworks with Paddle-Wheel SBUs upon Hydration*, **Chem. Mater.** 24, 3153 (2012) [10.1021/cm301427w](https://doi.org/10.1021/cm301427w). (IF: 10.1)
6. N. Nijem, **P. Canepa**, L. Kong, H. Wu, J. Li, T. Thonhauser and Y. J. Chabal, *Spectroscopic characterization of van der Waals interactions: Adsorbates in nanoporous materials*, **J. Phys.: Condens. Matter.** 24, 424203 (2012) [10.1088/0953-8984/24/42/424203](https://doi.org/10.1088/0953-8984/24/42/424203). (IF: 2.333)
5. **P. Canepa**, P. Ugliengo and M. Alfredsson, *Elastic and vibrational properties of α and β -PbO*, **J. Phys. Chem. C** 116, 21514 (2012) [10.1021/jp3036988](https://doi.org/10.1021/jp3036988). (IF: 4.126)
4. **P. Canepa**, E. Schofield, A. V. Chadwick and M. Alfredsson, *Comparison of calculated and measured XANES spectrum of α -Fe₂O₃*, **Phys. Chem. Chem. Phys.** 13, 12826 (2011) [10.1039/c1cp00034a](https://doi.org/10.1039/c1cp00034a). (IF: 4.123)

3. **P. Canepa**, R. M. Hanson, P. Ugliengo and M. Alfredsson, *J-ICE: a new Jmol interface for handling and visualizing crystallographic and electronic properties*, **J. Appl. Cryst.** 44, 225 (2011) [10.1107/S0021889810049411](https://doi.org/10.1107/S0021889810049411). (IF: 2.570)
2. **P. Canepa**, F. Chiatti, M. Corno, Y. Sakhno, G. Martra, and P. Ugliengo, *Affinity of hydroxyapatite (001) and (010) surfaces to formic and alendronic acids: a quantum-mechanical and infrared*, **Phys. Chem. Chem. Phys.** 13, 1099 (2011) [10.1039/c0cp01143f](https://doi.org/10.1039/c0cp01143f). (IF: 4.123)
1. **P. Canepa**, D. Kossoff, K. Hudson-Edwards, W. Dubbin and M. Alfredsson, *Hematite Contaminated by Heavy Metals*, **Geochim. Cosmochim. Ac.** 73, A189 (2009) [2009GeCAS.73Q.189C](https://doi.org/10.1016/S0016-7037(09)00189-0). (IF: 4.250)

Dissertations

2. **P. Canepa**, Ph.D. Dissertation Thesis: New insights on Iron and Lead-based materials beyond density functional theory, University of Kent (2012), Canterbury, Kent (UK). British Library <http://ethos.bl.uk/OrderDetails.do?uin=uk.bl.ethos.580391>.
1. **P. Canepa**, M.Sc. Dissertation Thesis: Acid dissolution of hydroxyapatite surfaces an Ab-initio approach. Title in Italian, Dissoluzione acida di superfici di idrossiapatite: un approccio *ab initio*, Università Degli Studi di Torino (2008), Italy <http://hdl.handle.net/2318/483>

Patentes & Inventions

2. *A Simple Metal-Organic Framework for The Selective Adsorption of Carbon Dioxide from Flue Gas*, D. Mullangi, Z. Deng, Y. Wang, J. Wang, **P. Canepa**, D. Zhao, A. K. Cheetham
1. *Electrode, Electrochemical Cell And Methods Of Forming The Same*, B. Özyilmaz, C. Cetin, C. T. Toh, I. H. Abidi, **P. Canepa**, X. F. Lim, PCT/SG2020/050551, [WO2021/066746 A1](https://patents.google.com/patent/WO2021/066746A1)

Consultancy

2021–present

Dyson Singapore Technology Centre.

Invited Talks & Seminars

51. 31st–May–2022 European-Materials Research Society, e-MRS, Spring 2022, Symposium R (Computations for Materials – Discovery, Design and the role of Data), Strasbourg, France

50. 12th–December–2021 14th Pacific Rim Conference on Ceramic and Glass Technology (PACRIM 14) including Glass & Optical Materials Division 2021 Annual Meeting (GOMD 2021), Vancouver, BC, Canada
49. 27st–November–2021, Colloquium at Pusan National University, Department of Chemistry, Pusan, Korea.
48. 6th–November–2021, A-0129 1st International Conference on Energy Materials (ICEM-XMUM VIRTUAL CONFERENCE 2021), 5th Anniversary of Xiamen University Malaysia and 100th Anniversary of Xiamen University (China).
47. May 30th to June 3rd–2021, 239th ECS Meeting with the 18th International Meeting on Chemical Sensors, Chicago, IL, USA.
46. 18th–April–2021 Materials Research Society, Spring, Seattle, WA, USA.
45. 14th–January–2021 Online symposium, Solving the Intricacies of NaSICON Electrolytes & Electrodes for Na-ion Batteries using Ab initio Methods, ShanghaiTech University, Shanghai, China.
44. 26th–November–2020 9th MRSS National Conference on Advanced Materials (MRSS AMC-9), Singapore, Singapore.
43. 5th–October–2020 Electrochemical Society Meeting PRiME 2020, Electrochemical Stability and Ionic Transport in Coating Materials for Mg Batteries A02-0212, Honolulu, HI, USA.
42. 5th–October–2020 Electrochemical Society Meeting PRiME 2020, Phase Behavior in Nasicon Electrolytes and Electrodes A05-1002, Honolulu, HI, USA.
41. 16th–September–2020 Israel National Research Center for Electrochemical Propulsion (INREP) Annual Conference 2020, Tel Aviv, Israel.
40. 12th–March–2020 International Battery Association 2020 (IBA), Bled, Slovenia.
39. 2nd–November–2019 10th ICMaSS2019 International Conference on Materials and Systems for Sustainability, Nagoya, Aichi, Japan.
38. 3st–October–2019 Seminar at University of New South Wales, Sydney, NSW, Australia.
37. 1st–October–2019 9th Conference of the Asia-Pacific Association of Theoretical and Computational Chemists (APATCC 2019), University of Sydney, Sydney, NSW, Australia.
36. 24th–July–2019, 2nd Global Forum on Advanced Materials and Technologies for Sustainable Development, Toronto, ON, Canada.
35. 22nd–July–2019, 2nd Global Forum on Advanced Materials and Technologies for Sustainable Development, Toronto, ON, Canada.
34. 10th–July–2019, The 11th International Conference on the Science and Technology for Advanced Ceramics, Tsukuba, Ibaraki, Japan.
33. 8th–July–2019, National Institute for Materials Science, Research Talk in the group of Dr. Yoshitaka Tateyama, Tsukuba, Ibaraki, Japan.
32. 25th–June–2019, International Conference on Materials for Advanced Technologies, Singapore.
31. 30th–May–2019, European-Materials Research Society, e-MRS, Nice, France.

30. 16th–January–2019, A*STAR Symposium beyond the Materials Genome, Fusionopolis, Singapore.
29. 27th–September–2018, 2nd International Symposium on Magnesium Batteries, Ulm, Germany.
28. 6th–April–2018, University College of London, United Kingdom.
27. 8th–March–2018, National University of Singapore, Singapore.
26. 4th–December–2017, TU Delft, The Netherlands.
25. 16th–September–2017, LRCS Amiens and Université de Picardie Jules Verne, France.
24. 21st–August–2017, XXIV International Materials Research Congress, Cancún, Mexico.
23. 6th–July–2017, University of Turin, Italy.
22. 12th–June–2017, Technische Universität Freiberg, Germany.
21. 31st–May–2017, University of Kent, Canterbury, UK.
20. 18th–May–2017, University of Birmingham, Birmingham, UK.
19. 22nd–March–2017, University of Cambridge, UK.
18. 24th–February–2017, University of Bath, UK.
17. 31st–August–2016, TACC Theory and Applications of Computational Chemistry, Seattle, WA, USA.
16. 10th–October–2015, 228th Electrochemical Society Meeting (ECS), Phoenix, AZ, USA.
15. 8th–April–2015, Materials Research Meeting (MRS), San Francisco, CA, USA.
14. 8th–January–2014, Joint Center for Energy Storage Research, JCSER, Bolingbrook, Chicago, IL, USA.
13. 28th–May–2013, Pacific North West National Laboratory, Richland, WA, USA.
12. 21st–May–2013, Ceder's Group, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Boston, MA, USA.
11. 29th–April–2013, WFU Physics Colloquium, Wake Forest University, Winston–Salem, NC, USA.
10. 21th–March–2013, *Chairman of Session U24: Focus Session: Recent Developments in Density Functional Theory III*, American Physical Society meetings, Baltimore, MD, USA.
9. 25th–February–2013, National Institute of Standards and Technology, Gaithersburg, MD, USA.
8. 5th–December–2012, WFU Physics Colloquium, Wake Forest University, Winston-Salem, NC, USA.
7. 27th–November–2012, Materials Research Meeting (MRS), Boston, MA, USA.
6. 21st–November–2012, School of Physical Science, University of Kent, Canterbury, UK.
5. 18th–June–2012, Materials Sciences and Technology Division, Oak Ridge National Laboratory, TN, USA.

4. 6th–June–2012, Electronic Structure Workshop ES12, Wake Forest University, Winston-Salem, NC, USA.
3. 25th–January–2012, University of Texas at Dallas (UTD), Richardson, TX, USA.
2. 31st–May–2011, Interreg IVB North Sea Region, University of Kent, Canterbury, UK.
1. 11th–January–2011, University of Turin, Italy.

Contributed Talks

1. 14th–September–2021, E4-15, Z. Deng, Phase Behaviour and its Relationship to Ion Mobilities of NaSiCON Electrolytes and Electrodes, EUROMAT 2021, Graz, Austria

Teaching Experience

Module Designed and/or Taught at NUS

- ▷ **Design and Teaching of the Module:** Atomistic modelling of molecules and materials, MLE5215/CN5215, 2019/2020 Semester #1, 2020/2021 Semester #1
- ▷ **Teaching:** Materials Engineering Principles & Practices, MLE1010, 2020 Semester #2, 2021 Semesters #1 & #2
- ▷ **Teaching:** Innovation Programme, EG2604, 2020 Semester #2
- ▷ **Teaching:** Design Project, MLE4102, 2019 Semester #1

University of Bath, UK

- ▷ Inorganic Chemistry, Class CH10133/134, Fall & Spring 2016 – 2017

Massachusetts Institute of Technology, USA

- ▷ Atomistic Computer Modeling of Materials, Class 3.320, Spring 2014 [Click here](#)

Student Supervision & Participation to Thesis Committees

Supervision of Ph.D. Students, NUS

1. Mr. Tara Prashad Mishra, 2018–present
2. Mr. Ziliang Wang, 2019–present
3. Ms. Hengning Chen, 2020–present
4. Mr. Tieu Jua (Aaron) Kang, 2021–present
5. Mr. Abhishek A. Panchal, 2021–present
6. Mr. Shidong Yu co-advised with Prof. Simon Redfern at NTU, 2020–present

Supervision of Postdoctoral Fellows & Research Engineers, NUS

1. Dr. Pandu Wisesa, 2021–present
2. Dr. Yuheng Li, 2021–present
3. Dr. Juefan Wang, 2021–present
4. Dr. Stephanie van der Lubbe, 2021–present
5. Mr. Timothy D. Pook (Research Engineer), 2021–present
6. Dr. Zeyu Deng, 2019–present
7. Dr. Baltej Singh Gill, 2019 August–2021 September, now research fellow at the University of Waterloo, Ontario, Canada, in Prof. Linda Nazar laboratory <http://www.science.uwaterloo.ca/~lfnazar/people.html#nazar>

Supervision of Master Students, NUS

1. Mr. Liang Bochun, 2020–2021. Now a Ph.D. student at the City University of Hong Kong in Prof. Jun Fan's laboratory <https://ourphysics.org/members/>

Supervision of Undergraduate, UROP and Final Year Project Students, NUS

1. Mr. Damien Lee Khai Jie, UROP student, 2021–present.
2. Mr. Niloy Faiyaz, FYP, (semester 2).
3. Mr. Yao Kuan, FYP, 2021 (semester 2).
4. Mr. Preston Lim, FYP, 2021 (semester 2).
5. Ms. Vishakha Kapoor, FYP, 2020–2021. **Best FYP Thesis of year 2021 in MSE.** Now a Research Assistant in MSE @ NUS in the Prof. Stefan Adams' laboratory <http://www.dmse.nus.edu.sg/asn/index.html>.
6. Mr. Wang Lu (Luis), FYP, 2020–2021. Now Trading Analyst at Glencore, PLC. <https://www.linkedin.com/in/wang-lu/>
7. Mr. Pengfei Cai, Undergraduate summer student, 2020.

Supervision of Visiting Students

1. Mr. Han Yunlu, from Shanghai Jiao Tong University, Shanghai, China, Sep. 2021–Jan. 2022.

Ph.D. Thesis Committees and Examination, NUS

1. Ms. He Wen, Ph.D. student in Physics, NUS, 18th October 2021.
2. Mr. Daniel Koch, Ph.D. student of Mechanical Engineering, NUS, 30th November 2020.
3. Ms. Juefan Wang, Ph.D. student in Physics, NUS, 5th November 2020.
4. Mr. Abhinav Tripathi, Ph.D. student of Mechanical Engineering, NUS, 11th November 2019.

Professional Activities

Referee's Activities

- ▷ **Nature X:** Nature Materials, Nature Energy, Nature Chemistry, Nature Commun. and npj Comp. Mat.
- ▷ **American Chemical Society:** Chemical Reviews, J. Amer. Chem. Soc., ACS Energy Lett., Nano Lett., Chem. Mater., J. Chem. Theory Comput., ACS Appl. Mater. Interfaces and J. Phys. Chem;
- ▷ **Royal Society of Chemistry:** Energy Environ. Sci., J. Mat. Chem. A, Phys. Chem. Chem. Phys. and RSC Adv;
- ▷ **Wiley:** Adv. Mater., Angew. Chem., Adv. Energy Mater., Adv. Func. Mater., Adv. Mater. Interfaces and Batteries & Supercaps;
- ▷ **Institute of Physics:** J. Electrochem. Soc;
- ▷ **American Physical Society:** Phys. Rev. B;
- ▷ **Elsevier:** Joule, Electrochim. Acta and Solid State Ion;

Proposal reviews

- ▷ **Singapore:** MOE-AcRF-Tier1 FRC-FY2021;
- ▷ **Europe:** ERC European Research Council; ERC starting grant; EPSRC Engineering and Physical Sciences Research Council (UK), ANR Agence nationale de la recherche; FWF Fonds zur Förderung der wissenschaftlichen Forschung Austrian Science Fund.; ÖWA Austrian Academy of Sciences; BSF Basic Research Funds Israel; NWO — Netherlands Organisation for Scientific Research;
- ▷ **South America:** National Fund for Scientific and Technological Development (FONDECYT) of the Chilean National Commission for Scientific and Technological Research.
- ▷ **Oceania:** Australian Nuclear Facility Organization (ANSTO).

Research in the News

1. **April 28, 2021** MIT News Office: SMART investigates the science behind varying performance of different colored LEDs. <https://news.mit.edu/2021/smart-performance-different-colored-leds-0428>
2. **April 13, 2021** AZOOptics: New Method may Lead to More Efficient LEDs. <https://www.azooptics.com/News.aspx?newsID=26731>
3. **April 12, 2021** ScienceDaily: SMART discovers the science behind varying performance of different colored LEDs. <https://www.sciencedaily.com/releases/2021/04/210412114745.htm>
4. **April 12, 2021** Semiconductor Today: New method observes compositional fluctuations in high-indium-content InGaN LEDs. http://www.semiconductor-today.com/news_items/2021/apr/smart-mit-120421.shtml
5. **April 12, 2021** NanoWerk: Researchers discover the science behind varying performance of different colored LEDs. <https://www.nanowerk.com/nanotechnology-news2/newsid=57762.php>

6. **September 28, 2020** Phys.org: Borate-based passivation layers enables reversible calcium batteries. <https://phys.org/news/2020-09-borate-based-passivation-layers-enables-reversible.html>
7. **September 28, 2020** NanoWerk: Borate-based passivation layers enable reversible calcium batteries. <https://www.nanowerk.com/nanotechnology-news2/newsid=56262.php>
8. **December 22, 2017** MaterialsToday: New solid-state conductor boosts magnesium-ion batteries. <https://www.materialstoday.com/energy/news/solidstate-conductor-magnesiumion-batteries/>
9. **December 28, 2017** Charged: DOE researchers announce major advance toward a solid-state magnesium battery. <https://chargedevs.com/category/newswire/the-tech/>
10. **November 28, 2017** Green Car Congress: JCESR team advances prospects of solid-state magnesium-ion batteries with discovery of fastest magnesium-ion solid-state conductor. <http://www.greencarcongress.com/2017/11/20171128-jcesr.html>
11. **November 28, 2017** Phys.org: 'Holy grail' for batteries: Solid-state magnesium battery a big step closer. <https://phys.org/news/2017-11-holy-grail-batteries-solid-state-magnesium.html>