

# David M. Halat

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## ACADEMIC PROFILE

### October 2018 — present

***University of California, Berkeley, Berkeley, CA, USA***

***and Lawrence Berkeley National Laboratory, Berkeley, CA, USA***

**Postdoctoral Scholar, Joint Center for Energy Storage Research (JCESR)**

Groups of Jeffrey A. Reimer and Nitash P. Balsara

Research focus: Electrophoretic NMR methods to probe ion transport and clustering in liquid and polymer electrolytes for Li-ion batteries

### January 2018 — October 2018

***University of Cambridge, Cambridge, UK***

**Post-doctoral Research Associate**

Group of Clare P. Grey, FRS

Research Associate, NorthEast Center for Chemical Energy Storage

Research focus: Solid-state NMR spectroscopic methods to characterize electrochemically-induced changes to the surface and bulk of layered transition-metal oxide Li-ion battery materials

### September 2013 — January 2018

***University of Cambridge, Cambridge, UK***

**PhD in Chemistry**

Supervisor: Clare P. Grey, FRS

Thesis:  $^{17}\text{O}$  Solid-State NMR Spectroscopy of Functional Oxides for Energy Conversion

Cambridge International Scholarship (2013 – 2016)

Researcher, NorthEast Center for Chemical Energy Storage (2016 – 2018)

### August 2009 — May 2013

***Montana State University, Bozeman, MT, USA***

**B.S. in Chemistry, *magna cum laude***

**B.S. in Mathematics, *magna cum laude***

Research supervisor: Robert A. Walker

Research thesis: Optical Studies of Solid Oxide Fuel Cell (SOFC) Anode Degradation and Failure

GPA: 4.0/4.0

## SELECTED HONORS AND AWARDS

- Highly Commended Thesis Prize, Dept. of Chemistry, Cambridge 2018
- IOP BRSG: Magnetic Resonance Group Founder's Prize 2016
- ECS Glasgow Sponsorship – Energy Storage Research Network 2015
- Dean's Award for Academic Excellence – Awarded to top two students in College of Letters and Science, Montana State 2013
- Barry M. Goldwater Scholarship – Awarded to top ~250 science/math/engineering students in USA 2012–2013
- Phi Kappa Phi Outstanding Student Award 2012
- Phi Kappa Phi Honor Society 2010
- Siemens Award for Advanced Placement (AP) – Awarded to top male and female AP students in each U.S. state 2009

## PUBLICATIONS

**29.** Rinkel, B. L. D.; **Halat, D. M.**; Griffith, K. J.; Hope, M. A.; Grey, C. P. Study of cation ordering and surface structure of  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  using  $^{17}\text{O}$  solid-state NMR spectroscopy; *in preparation* (2020).

**28.** Kerber, R. N.; Flint, S.; **Halat, D. M.**; Gaultois, M. W.; Grey, C. P. Oxygen vacancy formation in  $\text{CeO}_{2-\delta}$  and  $\text{Cu}_x\text{Ce}_{1-x}\text{O}_{2-\delta}$  bulk: a combined DFT and XRD study; *in preparation* (2020).

**27.** Mao, H.; Tang, J.; Peng, Y.; **Halat, D. M.**; Yang, A.; Xiao, L.; Lv, X.; Cui, Y.; Reimer, J. A. Large scale wood-derived carbon sphere/graphene membranes for efficient adsorption performance; *in revision* (2020).

**26.** Mozur, E. M.; Hope, M. A.; Trowbridge, J.; **Halat, D. M.**; Daemen, L. L.; Maughan, A. E.; Prisk, T. R.; Grey, C. P.; Neilson, J. R. Cesium Substitution Disrupts Concerted Cation Dynamics in Formamidinium Hybrid Perovskites; *Chem. Mater.*, *accepted* (2020).

**25.** Chen, J.; Hope, M. A.; Lin, Z.; Wang, M.; Liu, T.; **Halat, D. M.**; Wen, Y.; Chen, T.; Ke, X.; Magusin, P. C. M. M.; Ding, W.; Xia, X.; Wu, X-P.; Gong, X-Q.; Grey, C. P.; Peng, L. Interactions of Oxide Surfaces with Water Revealed with Solid-State NMR Spectroscopy. *J. Am. Chem. Soc.*, *in press* (2020).

**24.** Hope, M. A.; Zhang, B.; Zhu, B.; **Halat, D. M.**; MacManus-Driscoll, J. L.; Grey, C. P. Probing Interfaces in Complex Oxide Heterostructures via  $^{17}\text{O}$  Solid State NMR Spectroscopy; *ChemRxiv preprint* (2020).

**23.** Britto, S.; Seymour, I. D.; **Halat, D. M.**; Hidalgo, M. F. V.; Siu, C.; Reeves, P. J.; Zhou, H.; Chernova, N. A.; Whittingham, M. S.; Grey, C. P. Evolution of lithium ordering with (de)-lithiation in  $\beta\text{-LiVOPO}_4$ : insights through solid state NMR and first principles DFT calculations; *J. Mater. Chem. A* **8**, 5546–5557 (2020).

**22.** Choo, Y.; **Halat, D. M.**; Villaluenga, I.; Balsara, N. P. Diffusion and Migration in Polymer Electrolytes; *Prog. Polym. Sci.* **103**, 101220 (2020).

21. Jaffe, A.; Ziebel, M. E.; **Halat, D. M.**; Biggins, N.; Murphy, R. A.; Chakarawet, K.; Reimer, J. A.; Long, J. R. High-Temperature O<sub>2</sub> Adsorption in Chemically Reduced, Redox-Active Fe-Pyrazolate Metal–Organic Frameworks; *ChemRxiv preprint* (2019).
20. Chen, J.; Wu, X-P.; Hope, M. A.; Qian, K.; **Halat, D. M.**; Liu, T.; Jin, Y.; Zhao, E. W.; Li, Y.; Shen, L.; Ke, X.; Wen, Y.; Du, J-H.; Magusin, P. C. M. M.; Paul, S.; Yu, G.; Ding, W.; Gong, X-Q.; Grey, C. P.; Peng, L. Polar Surface Structure of Oxide Nanocrystals Revealed with Solid-State NMR Spectroscopy; *Nat. Comm.* **10**, 1–10 (2019).
19. Lebens-Higgins, Z. W.; **Halat, D. M.**; Faenza, N. V.; Wahila, M. J.; Mascheck, M.; Wiell, T.; Eriksson, S. K.; Palmgren, P.; Rodriguez, J.; Badway, F.; et al. Surface Chemistry Dependence on Aluminum Doping in Ni-Rich LiNi<sub>0.8</sub>Co<sub>0.2-y</sub>Al<sub>y</sub>O<sub>2</sub> Cathodes. *Sci. Rep.* **9**:17720 (2019).
18. **Halat, D. M.**; Britto, S.; Griffith, K. J.; Jónsson, E.; Grey, C. P. Natural abundance solid-state <sup>33</sup>S NMR study of NbS<sub>3</sub>: applications for battery conversion electrodes; *ChemComm* **55**, 12687–12690 (2019).
17. Hope, M. A.; **Halat, D. M.**; Lee, J.; Grey, C. P. A <sup>17</sup>O Paramagnetic NMR Study of Sm<sub>2</sub>O<sub>3</sub>, Eu<sub>2</sub>O<sub>3</sub>, and Sm/Eu-substituted CeO<sub>2</sub>; *Sol. State Nucl. Magn. Reson.*, **102**, 21–30 (2019). **Cover article** for themed paramagnetic NMR issue.
16. Galluzzo, M. D.; **Halat, D. M.**; Loo, W. S.; Mullin, S. A.; Reimer, J. A.; Balsara, N. P. Dissolution of Lithium Metal in Poly(ethylene oxide); *ACS Energy Lett.*, **4**, 903–907 (2019).
15. Dunstan, M. T.\*; **Halat, D. M.\***; Tate, M. L.; Evans, I. R.; Grey, C. P. Variable-temperature multinuclear solid-state NMR study of oxide ion dynamics in fluorite-type bismuth vanadates and phosphates; *Chem. Mater.*, **31**, 1704–1714 (2019). (\* = equal contribution)
14. Faenza, N. V.; Pereira, N.; **Halat, D. M.**; Vinckeviciute, J.; Bruce, L.; Radin, M. D.; Mukherjee, P.; Badway, F.; Halajko, A.; Cosandey, F.; Grey, C. P.; Van der Ven, A.; Amatucci, G. G. The Phase Evolution and Degradation Modes of *R*-3*m* Li<sub>x</sub>Ni<sub>1-y-z</sub>Co<sub>y</sub>Al<sub>z</sub>O<sub>2</sub> Electrodes Cycled Near Complete Delithiation; *Chem. Mater.*, **30**, 7545–7574 (2018).
13. Wu, Y.; **Halat, D. M.**; Wei, F.; Binford, T.; Seymour, I. D.; Gaultois, M. W.; Shaker, S.; Wang, J.; Grey, C. P.; Cheetham, A. K. Mixed X-Site Formate–Hypophosphite Hybrid Perovskites. *Chem. Eur. J.* **24**, 11309–11313 (2018).
12. **Halat, D. M.**; Dunstan, M. T.; Gaultois, M. W.; Grey, C. P. Study of Defect Chemistry in the System La<sub>2-x</sub>Sr<sub>x</sub>NiO<sub>4+δ</sub> by <sup>17</sup>O Solid-State NMR Spectroscopy and Ni K-Edge XANES. *Chem. Mater.* **30**, 4556–4570 (2018).
11. Lebens-Higgins, Z. W.; Sallis, S.; Faenza, N. V.; Badway, F.; Pereira, N.; **Halat, D. M.**; Wahila, M.; Schlueter, C.; Lee, T.-L.; Yang, W.; Grey, C. P.; Amatucci, G. G.; Piper, L. F. J. Evolution of the Electrode–Electrolyte Interface of LiNi<sub>0.8</sub>Co<sub>0.15</sub>Al<sub>0.05</sub>O<sub>2</sub> Electrodes Due to Electrochemical and Thermal Stress. *Chem. Mater.*, **30**, 958–969 (2018).
10. Kim, G.; Griffin, J. M.; Blanc, F.; **Halat, D. M.**; Haile, S. M.; Grey, C. P. Revealing Local Dynamics of the Protonic Conductor CsH(PO<sub>3</sub>H) by Solid-State NMR Spectroscopy and First-Principles Calculations. *J. Phys. Chem. C*, **121**, 27830–27838 (2017).
9. Hope, M. A.; **Halat, D. M.**; Magusin, P. C. M. M.; Paul, S.; Peng, L.; Grey, C. P. Surface-selective direct <sup>17</sup>O DNP NMR of CeO<sub>2</sub> nanoparticles. *ChemComm* **53**, 2142–2145 (2017).

8. Pecher, O.\*; **Halat, D. M.\***; Lee, J.; Liu, Z.; Griffith, K. J.; Braun, M.; Grey, C. P. Enhanced efficiency of solid-state NMR investigations of energy materials using an external automatic tuning/matching (eATM) robot. *J. Magn. Reson.* **275**, 127–136 (2017). (\* = equal contribution)
7. **Halat, D. M.**; Dervişoğlu, R.; Kim, G.; Dunstan, M. T.; Blanc, F.; Middlemiss, D. S.; Grey, C. P. Probing Oxide-Ion Mobility in the Mixed Ionic–Electronic Conductor  $\text{La}_2\text{NiO}_{4+\delta}$  by Solid-State  $^{17}\text{O}$  MAS NMR Spectroscopy. *J. Am. Chem. Soc.* **138**, 11958–11969 (2016).
6. Seymour, I. D.; Middlemiss, D. S.; **Halat, D. M.**; Trease, N. M.; Pell, A. J.; Grey, C. P. Characterizing Oxygen Local Environments in Paramagnetic Battery Materials via  $^{17}\text{O}$  NMR and DFT Calculations. *J. Am. Chem. Soc.* **138**, 9405–9408 (2016).
5. Reeping, K. W.; **Halat, D. M.**; Kirtley, J. D.; McIntyre, M. D.; Walker, R. A. *In Situ* Optical and Electrochemical Studies of SOFC Carbon Tolerance. *ECS Trans.* **61**, 57–63 (2014).
4. McIntyre, M. D.; Kirtley, J. D.; **Halat, D. M.**; Reeping, K. W.; Walker, R. A. *In Situ* Spectroscopic Studies of Carbon Formation in SOFCs Operating with Syn-gas. *ECS Trans.* **57**, 1267–1275 (2013).
3. Kirtley, J. D.; McIntyre, M. D.; **Halat, D. M.**; Walker, R. A. Insights into SOFC Ni/YSZ Anode Degradation Using *In-Situ* Spectrochronopotentiometry. *ECS Trans.* **50**, 3–15 (2013).
2. Kirtley, J.; Singh, A.; **Halat, D.**; Oswell, T.; Hill, J. M.; Walker, R. A. *In Situ* Raman Studies of Carbon Removal from High Temperature Ni–YSZ Cermet Anodes by Gas Phase Reforming Agents. *J. Phys. Chem. C* **117**, 25908–25916 (2013).
1. Kirtley, J. D.; **Halat, D. M.**; McIntyre, M. D.; Eigenbrodt, B. C.; Walker, R. A. High-Temperature ‘Spectrochronopotentiometry’: Correlating Electrochemical Performance with *In Situ* Raman Spectroscopy in Solid Oxide Fuel Cells. *Anal. Chem.* **84**, 9745–9753 (2012).

## RESEARCH EXPERIENCE

### October 2018 — present

**Postdoctoral Scholar** with Prof. Jeffrey A. Reimer, Department of Chemical and Biomolecular Engineering, University of California, Berkeley and Prof. Nitash P. Balsara, Materials Science Division, Lawrence Berkeley National Laboratory (Berkeley, CA, USA)

- Developing and applying novel electrophoretic, variable-temperature NMR methods to study ion transport, dynamics, and clustering of ionic liquids dissolved in solid polymer electrolyte materials for Li-ion batteries
- Using solid-state NMR techniques for the characterization of structure, phase purity, and dissolution/adsorption properties of solid polymer electrolytes, porous anionic frameworks, and metal organic frameworks
- Applying pulsed-field gradient (PFG) NMR for measuring long-range ionic diffusion in ionic liquids and polymer electrolytes

### **January 2018 — October 2018**

**Post-doctoral Research Associate** with Prof. Clare P. Grey FRS, Department of Chemistry, University of Cambridge (Cambridge, UK)

- Used advanced solid-state NMR methods (*e.g.* REDOR, TRAPDOR) to study the composition and formation of the electrode–electrolyte interphase at paramagnetic lithium-ion battery cathode materials such as NCA ( $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ )

### **September 2013 — January 2018**

**Postgraduate Researcher** with Prof. Clare P. Grey FRS, Department of Chemistry, University of Cambridge (Cambridge, UK)

- Performed solid-state synthesis and characterization of oxide-ion conducting materials (*e.g.*,  $\text{La}_2\text{NiO}_{4+\delta}$ ) for solid oxide fuel cells (SOFC), oxygen sensor and chemical looping applications
- Developed  $^{17}\text{O}$  solid-state NMR spectroscopy techniques (advanced pulse sequences, variable-temperature measurements up to  $800^\circ\text{C}$ ) for paramagnetic materials
- Extended theoretical methodology for calculating NMR shifts of paramagnetic transition metal oxides, and simulated spectra influenced by ion dynamics
- Gained experience in multinuclear and high-field NMR studies ( $^6/7\text{Li}$ ,  $^{11}\text{B}$ ,  $^{19}\text{F}$ ,  $^{27}\text{Al}$ ,  $^{31}\text{P}$ ,  $^{33}\text{S}$ ,  $^{51}\text{V}$ ,  $^{67}\text{Zn}$ ,  $^{183}\text{W}$ ) relevant for energy conversion/storage systems
- Developed and tested external automatic tuning matching (eATM) robot to enhance efficiency in acquiring broad solid-state NMR spectra, *e.g.* of paramagnetic systems, in collaboration with NMR Service GmbH (Erfurt, DE)
- Advanced direct dynamic nuclear polarization (DNP) NMR as a tool to selectively probe and distinguish surfaces of catalytic oxide nanoparticles

### **January 2011 — August 2013**

**Undergraduate Researcher** with Prof. Robert A. Walker, Department of Chemistry and Biochemistry, Montana State University (Bozeman, MT, USA)

- Investigations of operational SOFCs with simultaneous *in situ* vibrational Raman spectroscopy and electrochemistry, including electrochemical impedance spectroscopy (EIS), at high temperature ( $600\text{--}800^\circ\text{C}$ )
- Designed custom SOFC rig for studies of anode-supported cells

### **Academic and laboratory visits:**

#### **July — August 2014**

**Visiting** the laboratory of Clare P. Grey, FRS at SUNY Stony Brook

- Performed variable-temperature NMR of oxide-ion conductors to understand high-temperature ion dynamics
- Gained experience with Agilent/Varian NMR systems and Spinsight software

#### **May — June 2012**

**Visiting researcher** with Dr. Gregory Offer and Prof. Nigel Brandon OBE FEng, Department of Earth Sciences and Engineering, Imperial College (London, UK)

- Investigated solid oxide fuel cell (SOFC) performance and durability with micro-SOFC rig
- Performed comparative analysis of graphite formation on SOFCs under different electrochemical operating conditions and temperatures

#### **SELECTED PRESENTATIONS** (# Poster, \* Oral)

- "*Ion motion in the wrong direction: electrophoretic NMR of electrolytes for Li-ion batteries.*" \* Seminar at Lawrence Livermore National Laboratory, 30 January 2020, Livermore, CA, USA.
- "*Natural Abundance Solid-state  $^{33}\text{S}$  NMR Study of  $\text{NbS}_3$ : Applications for Battery Conversion Electrodes.*" # North American Solid State Chemistry Conference, 31 July 2019, Golden, CO, USA.
- "*Electrophoretic NMR studies of ion transport in solid polymer electrolytes.*" # 60<sup>th</sup> Experimental Nuclear Magnetic Resonance Conference, 9 April 2019, Asilomar, CA, USA.
- "*Natural Abundance Solid-state  $^{33}\text{S}$  NMR Study of  $\text{NbS}_3$ : Applications for Battery Conversion Electrodes.*" \* 60<sup>th</sup> Experimental Nuclear Magnetic Resonance Conference, 8 April 2019, Asilomar, CA, USA.
- "*Understanding local structure and oxide-ion dynamics in functional paramagnetic oxides using  $^{17}\text{O}$  solid-state NMR.*" # 59<sup>th</sup> Rocky Mountain Conference on Magnetic Resonance, 24 July 2018, Snowbird, UT, USA.
- "*Surface Selective  $^{17}\text{O}$  DNP NMR of  $\text{CeO}_2$  Nanoparticles.*" \* 10<sup>th</sup> Alpine Conference on Solid-State NMR, 13 September 2017, Chamonix, France. (Co-presented with Michael A. Hope, University of Cambridge.)
- "*Understanding local structure and oxide-ion dynamics in functional paramagnetic oxides using  $^{17}\text{O}$  solid-state NMR.*" \* 21<sup>st</sup> International Conference on Solid State Ionics, 23 June 2017, Padua, Italy.
- **Invited** – " *$^{17}\text{O}$  solid-state NMR of functional paramagnetic oxides for energy conversion and catalysis.*" \* IoP BRSG (Magnetic Resonance Group) Christmas Meeting, 14 December 2016, RIBA, London, UK. **Won Founder's Prize.**
- "*Oxide-Ion Dynamics in Paramagnetic  $\text{La}_2\text{NiO}_{4+\delta}$  by Experimental and Computational  $^{17}\text{O}$  NMR.*" # RSC Materials Chemistry Division Poster Symposium, 25 November 2016, Burlington House, London, UK.
- " *$^{17}\text{O}$  solid-state NMR spectroscopy of functional paramagnetic oxides.*" \* Materials RIG BP Day, 25 October 2016, Department of Chemistry, University of Cambridge, Cambridge, UK.
- "*Going paramagnetic:  $^{17}\text{O}$  NMR spectroscopy of functional paramagnetic oxides for energy storage, conversion and catalysis.*" \* DGK's Young Crystallographers Meeting, 22 September 2016, Humboldt University Berlin, Berlin, Germany.

- **Invited** – "*Paramagnetic  $^{17}\text{O}$  NMR as a sensitive probe of local structure and dynamics in mixed oxide-ionic–electronic conductors.*" \* Solid State Seminar, 6 May 2016, Inorganic Chemistry Laboratory, University of Oxford, Oxford, UK.
- "*Oxide-Ion Dynamics in the SOFC Cathode Material  $\text{La}_2\text{NiO}_{4+\delta}$  by Experimental and Computational Solid-State  $^{17}\text{O}$  NMR Spectroscopy.*" # Solid Oxide Fuel Cells XIV (SOFC-XIV), July 2015, Glasgow, UK.
- "*Oxide-ion dynamics in the MIEC SOFC cathode material  $\text{La}_2\text{NiO}_{4+\delta}$  by experimental and computational solid-state  $^{17}\text{O}$  NMR spectroscopy.*" \* 20<sup>th</sup> International Conference on Solid State Ionics, 15 June 2015, Keystone, CO, USA.
- "*Oxide-ion dynamics in the MIEC SOFC cathode material  $\text{La}_2\text{NiO}_{4+\delta}$  by experimental and computational solid-state  $^{17}\text{O}$  NMR.*" # STFC Early Career Researchers Conference, 8 March 2015, Abingdon, UK.
- "*Oxide-ion dynamics in the MIEC SOFC cathode material  $\text{La}_2\text{NiO}_{4+\delta}$  by experimental and computational solid-state  $^{17}\text{O}$  NMR.*" # H2FC Supergen (Hydrogen & Fuel Cell Researcher Conference), 15-17 December 2014, University of Birmingham, Birmingham, UK.
- "*Dynamic when hot: oxide-ion conduction in  $\text{La}_2\text{NiO}_{4+\delta}$  by experimental and computational  $^{17}\text{O}$  NMR.*" \* Materials RIG PhD Student Talks, 11 November 2014, Department of Chemistry, University of Cambridge, Cambridge, UK.
- "*Study of  $\text{La}_2\text{NiO}_{4+\delta}$ , a prospective SOFC cathode material, by computational and experimental  $^{17}\text{O}$  VT-NMR.*" # European Materials Research Society Spring Meeting 2014, 26-30 May 2014, Lille, France.
- "*In Situ Optical Studies of Solid Oxide Fuel Cells: SOFC Assembly with Concurrent Electrochemistry & Raman (SAwCER).*" (with Kyle W. Reeping.) # OpTeC Conference, 16 August 2013, Bozeman, MT, USA.
- "*In situ vibrational Raman spectroscopy as an analytical tool for studying the chemistry of solid oxide fuel cell (SOFC) processes.*" # 245<sup>th</sup> National Meeting of the American Chemical Society, 7-11 April 2013, New Orleans, LA, USA.
- "*In situ optical studies of carbon accumulation and persistence on Sn-impregnated Ni-YSZ cermet anodes in operational solid oxide fuel cells.*" \* OpTeC Conference, 17 August 2012, Bozeman, MT, USA.

## ORGANIZATIONAL ACTIVITIES

- 2018–** Lead of Joint Center for Energy Storage Research Association of Students and Postdocs (JCESR ASAP), and Representative to DOE Basic Energy Sciences Early Career Network
- 2017–2018** Group meeting coordinator (Grey Group, Cambridge) — scheduling and hosting internal group meetings, as well as talks given by external visitors
- 2016–2018** Group representative for ARCHER (UK National Supercomputing Service) — submission and defense of proposals for supercomputing time
- 2014–2016** Volunteer organizer for Chemistry Open Days, Department of Chemistry, University of Cambridge

- 2012–2013** Councilman of the Undergraduate Advisory Council, Dept. of Mathematical Sciences, Montana State University — budget advising role
- 2010–2013** Secretary (2010–11) and President (2012–13) of the Algebraic Adventurers (Montana State University Math Club) — seminar coordination, tutoring, math contest preparation
- 2010–2013** Member and volunteer for the Undergraduate Chemistry Society, Montana State University — community outreach activities, course mentoring, fundraisers
- Peer Review** Reviewer for *Angewandte Chemie* (2014), *Journal of the American Chemical Society* (2016), *Solid State Ionics* (2017), *Journal of Materials Chemistry A* (2019)

## TEACHING EXPERIENCE

- 2017–2018** Supervisor – PhD Student, Department of Chemistry, University of Cambridge
- 2016–2017** Supervisor – Master’s (Part III) Student, Department of Chemistry, University of Cambridge
- 2014–2015** Supervisor – Master’s (Part III) Student, Department of Earth Sciences, University of Cambridge
- 2014–2015** Demonstrator for Part IB (second-year) physical chemistry practicals in the Department of Chemistry, University of Cambridge
- 2013–2014** Demonstrator for Part IA (first-year) chemistry practicals in the Department of Chemistry, University of Cambridge

## COMPETITIONS

- William Lowell Putnam Mathematical Competition (2010\*, 2011, 2012)
  - \* In top 10% of competing students
- Honorable Mention, COMAP Mathematical Contest in Modeling (2011)

## TECHNICAL (COMPUTING) SKILLS

- Experience with computational chemistry (DFT) software
  - Gaussian, CASTEP, CRYSTAL, VASP
- Experienced in \*nix command line and shell scripting; knowledge of programming in TCL, Java, JavaScript, MATLAB, Python, Visual Basic, Maple;; experience with automated data analysis using IGOR Pro
- Acquisition and automated processing of NMR data using TopSpin, including pulse programming and development of native Python scripts
- Use of high-performance computing facilities (PBS and SLURM systems)
  - Darwin (University of Cambridge)
  - NANO (Center for Functional Materials, Brookhaven National Laboratory)
  - ARCHER (UK National Supercomputing Service)
  - TIGER cluster (College of Chemistry, UC Berkeley)