

Alexander Buhse Brady

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Employment

Oak Ridge National Laboratory Post-Doctoral Researcher, Geochemistry and Interfacial Sciences Advisors: Hsiu-Wen Wang, Andrew Stack	Oak Ridge, TN Oct 2018 – Present
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Education

Stony Brook University Materials Science and Chemical Engineering Advisors: Esther S. Takeuchi, Amy C. Marschilok, Kenneth J. Takeuchi	Stony Brook, NY Aug 2013 – Aug 2018
Cornell University B.S. in Electrical and Computer Engineering	Ithaca, NY Aug 2009 – May 2013

Awards/Honors

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| • Stony Brook Graduate Council Fellowship | 2013-2017 |
| • Cornell University Dean's List | 2009-2011 |

Research Experience

Postdoc in X-Ray Scattering Oak Ridge National Lab	Oak Ridge, TN	Oct 2018 – Present
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- Collected *in situ* SAXS and WAXS diffraction of BaSO₄ deposition on a porous silica substrate.
- Combining neutron diffraction and molecular dynamics modelling to study sodium ion intercalation into MXene structures.
- Created new procedures for data reduction and combined modelling approaches.
- Measured the solvation structure around sulfate and chlorine ions with combined neutron diffraction isotope substitution (NDIS) and molecular dynamics modelling.
- Created PDF models for Ti₃CN and Ti₃C₂ MXenes using DISCUS and Python.
- Measured the structure changes of titanium carbides *in situ* with x-ray diffraction upon intercalation with various cations.
- Group lead for FIRST EFRC junior scientist A-Team.
- Co-mentored two undergraduate students for summer of 2019, including trips to APS beamlines.

Research Assistant Stony Brook University	Stony Brook, NY	June 2013 – Aug 2018
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- Created PDF models of Ag_xMn₈O₁₆ and ZnFe₂O₄.
- Developed a stacking faulted model for AgFe₂O₄ and simulated structure in DIFFaX.
- Created Rietveld Refinement models of numerous materials in pristine and lithiated conditions, including Ag_xMn₈O₁₆, Li_{1+x}V₃O₈, CuFe₂O₄, AgFe₂O₄, Ag₂VOPO₄, and ZnFe₂O₄.
- Collected and analyzed experimental diffraction data, both on lab-scale X-Ray machines and at synchrotron light sources. Performed calibration for over 200 samples collected at the XPD (28-ID) beamline at NSLS-II, in addition to running samples at numerous other beamlines.
- Analyzed neutron diffraction data collected via mail-in from POWGEN at ORNL.
- Ran a conductivity study using two and four point methods, of Ag₂VO₂PO₄ and Fe₃O₄. Characterized the effect of pellet composition, pressing, and annealing conditions on conductivity.
- Simulated alpha-MnO₂ and LiV₃O₈ systems with DFT (density functional theory) modeling, using the software VASP and Siesta.

- Characterized the electrochemical behavior of many materials, especially polypyrrole and $\text{Ag}_2\text{VO}_2\text{PO}_4$, using cyclic voltammetry and galvanostatic cycling measurements.
- Synthesized Ag_2VOPO_4 and $\text{Ag}_2\text{VP}_2\text{O}_8$ using hydrothermal and solid state methods.
- Synthesized Fe_3O_4 and polypyrrole by electrodeposition. Mentored undergraduate researchers to test the effect of varied synthetic conditions (pH, current, voltage, and reactant concentration).
- Co-mentored three undergraduate students in summer of 2017.

Publications

1. Transition Metal Substitution of Hollandite α - MnO_2 : Enhanced Potential and Structural Stability on Lithiation from First Principles Calculation, **AB Brady**, KR Tallman, ES Takeuchi, AC Marschilok, KJ Takeuchi, P Liu, *Journal of Physical Chemistry C*, 123 (41), 25042-25051 (2019)
2. Energy-Dispersive X-ray Diffraction: Operando Visualization of Electrochemical Activity of Thick Electrodes, AM Bruck, L Wang, **AB Brady**, DM Lutz, BL Hoff, KLi, N Stavinski, DC Bock, KJ Takeuchi, ES Takeuchi, AC Marschilok, *Journal of Physical Chemistry C* 123 (31), 18834-18843 (2019)
3. Tomographic 3D Analysis of Reduction Displacement Reaction with Associated Formation of a Conductive Network in High Energy Primary Batteries, AM Bruck, YR Li, **AB Brady**, AC Chuang, JS Okasinski, KJ Takeuchi, ES Takeuchi, AC Marschilok, *Journal of the Electrochemical Society* 166 (14), A3210-A3216 (2019)
4. Temporally and Spatially Resolved Visualization of Electrochemical Conversion: Monitoring Phase Distribution During Lithiation of Magnetite (Fe_3O_4) Electrodes, AM Bruck, NW Brady, CN Lininger, DC Bock, **AB Brady**, KR Tallman, CD Quilty, KJ Takeuchi, ES Takeuchi, AC West, AC Marschilok, *ACS Applied Energy Materials* 2 (4), 2561-2569 (2019)
5. Investigation of α - MnO_2 Tunneled Structures as Model Cation Hosts for Energy Storage, LM Housel, L Wang, A Abraham, J Huang, GD Renderos, CD Quilty, **AB Brady**, AC Marschilok, KJ Takeuchi, ES Takeuchi, *Accounts of Chemical Research* 51 (3), 575-582 (2018)
6. Capacity Retention for (De) lithiation of Silver Containing α - MnO_2 : Impact of Structural Distortion and Transition Metal Dissolution, J Huang, LM Housel, CD Quilty, **AB Brady**, PF Smith, A Abraham, MR Dunkin, DM Lutz, B Zhang, ES Takeuchi, AC Marschilok, KJ Takeuchi, *Journal of the Electrochemical Society* 165 (11), A2849-A2858 (2018)
7. The Effect of Silver Ion Occupancy on Hollandite Lattice Structure, **AB Brady**, J Huang, JL Durham, PF Smith, J Bai, ES Takeuchi, AC Marschilok, KJ Takeuchi, *MRS Advances* 3 (10), 547-552 (2018)
8. Unveiling the Structural Evolution of $\text{Ag}_{1.2}\text{Mn}_8\text{O}_{16}$ under Coulombically Controlled (De) Lithiation, J Huang, X Hu, **AB Brady**, L Wu, Y Zhu, ES Takeuchi, AC Marschilok, KJ Takeuchi, *Chemistry of Materials* 30 (2), 366-375 (2018)
9. Deliberately Designed Atomic-Level Silver Containing Inter-phase Results in Improved Rate Capability and Utilization of Silver Hollandite for Lithium-Ion Storage, PF Smith, **AB Brady**, SY Lee, AM Bruck, E Dooryhee, L Wu, Y Zhu, KJ Takeuchi, ES Takeuchi, AC Marschilok, *ACS Applied Materials & Interfaces* (2017)
10. Probing the Li Insertion Mechanism of ZnFe_2O_4 in Li-Ion Batteries: A Combined X-Ray Diffraction, Extended X-Ray Absorption Fine Structure, and Density Functional Theory Study, Y Zhang, CJ Pelliccione, **AB Brady**, H Guo, PF Smith, P Liu, AC Marschilok, KJ Takeuchi, ES Takeuchi, *Chemistry of Materials* 29 (10), 4282-4292 (2017)
11. Investigation of Structural Evolution of $\text{Li}_{1.1}\text{V}_3\text{O}_8$ by In Situ X-ray Diffraction and Density Functional Theory Calculations, Q Zhang, **AB Brady**, CJ Pelliccione, DC Bock, AM Bruck, J Li, V Sarbada, R Hull, EA Stach, KJ Takeuchi, ES Takeuchi, P Liu, AC Marschilok, *Chemistry of Materials* 29 (5), 2364-2373 (2017)
12. Hybrid $\text{Ag}_2\text{VO}_2\text{PO}_4/\text{CF}_x$ as a High Capacity and Energy Cathode for Primary Batteries, YR Li, AM Bruck, **AB Brady**, D Bock, KJ Takeuchi, ES Takeuchi, AC Marschilok, *Journal of The Electrochemical Society* 164 (12), A2457-A2467 (2017)
13. Electrochemical (de) lithiation of silver ferrite and composites: mechanistic insights from ex situ, in situ, and operando X-ray techniques, JL Durham, **AB Brady**, CA Cama, DC Bock, CJ Pelliccione, Q Zhang,

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- M Ge, YR Li, Y Zhang, H Yan, X Huang, Y Chu d, ES Takeuchi, KJ Takeuchi, AC Marschilok, *Physical Chemistry Chemical Physics* 19 (33), 22329-22343 (2017)
14. Lithium Vanadium Oxide ($\text{Li}_{1.1}\text{V}_3\text{O}_8$) Coated with Amorphous Lithium Phosphorous Oxynitride (LiPON): Role of Material Morphology and Interfacial Structure on Resulting Electrochemistry, Q Zhang, AK Kercher, GM Veith, V Sarbada, **AB Brady**, J Li, EA Stach, R Hull, KJ Takeuchi, ES Takeuchi, NJ Dudney, AC Marschilok, *Journal of The Electrochemical Society* 164 (7), A1503-A1513 (2017)
 15. Magnesium-ion battery-relevant electrochemistry of MgMn_2O_4 : crystallite size effects and the notable role of electrolyte water content, J Yin, **AB Brady**, ES Takeuchi, AC Marschilok, KJ Takeuchi, *Chemical Communications* 53 (26), 3665-3668 (2017)
 16. Electrode Reaction Mechanism of $\text{Ag}_2\text{VO}_2\text{PO}_4$ Cathode, R Zhang, TA Abtew, NF Quackenbush, LW Wangoh, M Huie, **AB Brady**, D Bock, H Efstathiadis, MS Whittingham, AC Marschilok, KJ Takeuchi, ES Takeuchi, P Zhang, LFJ Piper, *Chemistry of Materials* 28 (10), 3428-3434 (2016)
 17. Redox chemistry of a binary transition metal oxide (AB_2O_4): a study of the $\text{Cu}_{2+}/\text{Cu}_0$ and $\text{Fe}_{3+}/\text{Fe}_0$ interconversions observed upon lithiation in a CuFe_2O_4 battery using X-ray absorption spectroscopy, CA Cama, CJ Pelliccione, **AB Brady**, J Li, EA Stach, J Wang, J Wang, ES Takeuchi, KJ Takeuchi, AC Marschilok, *Physical Chemistry Chemical Physics* 18 (25), 16930-16940 (2016)
 18. Structural Defects of Silver Hollandite, Ag_xMnsO_y , Nanorods: Dramatic Impact on Electrochemistry, L Wu, F Xu, Y Zhu, **AB Brady**, J Huang, JL Durham, E Dooryhee, AC Marschilok, ES Takeuchi, and KJ Takeuchi, *ACS Nano* 9 (8), 8430-8439 (2015)
 19. Electrochemical reduction of an $\text{Ag}_2\text{VO}_2\text{PO}_4$ particle: dramatic increase of local electronic conductivity, KC Kirshenbaum, DC Bock, **AB Brady**, AC Marschilok, KJ Takeuchi, ES Takeuchi, *Physical Chemistry Chemical Physics* 17 (17), 11204-11210 (2015)
 20. Synchrotron Enabled Ex-Situ and in-Situ Mechanistic Interrogation of Energy Storage Systems, **AB Brady**, K Kirshenbaum, KJ Takeuchi, AC Marschilok, ES Takeuchi, *ECS Transactions* 61 (18), 1-8 (2014)
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Presentations

1. AB Brady, *Stacking Faults in Layered Electrode Materials: Developments in Structure Solutions for Diffraction Data*. Oral presentation at the annual meeting of the American Crystallographic Association, 2019, Covington, Kentucky
 2. AB Brady, *The Use of Ex Situ, In Situ, and Operando X-Ray Diffraction to Understand Rate-Dependent Phenomena in Energy Storage Materials and Systems*. Oral presentation at the fall meeting of the Materials Research Society, 2017, Boston, Massachusetts
 3. AB Brady, *High Resolution X-ray Analysis and Complementary Spectroscopy to Describe the Structures and Function of Crystallographically Imperfect, Composite Energy Storage Materials*. Poster presented at the fall meeting of the Materials Research Society, 2017, Boston, Massachusetts
 4. AB Brady, *Structural Defects of Silver Hollandite, Ag_xMnsO_y , Nanorods: Dramatic Impact on Electrochemistry*. Poster presented at the Energy Frontier Research Centers PI meeting, 2015, Washington, DC
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Expertise and Skills

- **X-ray Crystallography:** GSAS I and II, TOPAS, DISCUS, Fullprof, PDFgetX3, PDFgetN, PDFGUI, VESTA, Mercury, CrystalMaker, CrystalDiffact
 - **Data analysis:** Rietveld analysis using GSAS, Matlab, Zview, PeakFit, PDXL released by Rigaku, ImageJ, Microsoft Word, Excel and PowerPoint
 - **Beamline Experiences:** XPD beamline at NSLSII at Brookhaven National Laboratory (Multiple Dates), EDXRD at Advanced Photon Source (APS) at Argonne National Laboratory (ANL) (Date); XAS experiment at APS (Date), Hard X-ray Nanoprobe (HXN) at NSLS-II (BNL), powder and liquid diffraction at POWGEN and NOMAD at SNS (ORNL).
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- **Characterization Methods:** XRD, thermogravimetric/calorimetric analysis (TGA/DSC), Scanning electron microscopy (SEM), inductively coupled plasma optical emission spectroscopy (ICP–OES), Brunauer–Emmett–Teller (BET) surface area and porosity measurements.
 - **Chemical Modeling:** Density Functional Theory (DFT) using VASP and SIESTA. Classical molecular dynamics in LAMMPS.
 - **Programming:** Matlab, Python (Numpy and Scipy), C, PHP, Java, Labview, Perl
 - **Battery systems:** Coating electrode and pellet electrode preparation, Karl Fischer titration, Assembling and de-assembling Li and Na coin cells, T-cells, Pouch cells
 - **Electrochemistry:** Cyclic Voltammetry, Galvanostatic cycling, Electrochemical impedance spectroscopy (EIS), Four-point probe
 - **Synthesis:** Hydrothermal, solid state
 - **Language:** Intermediate Chinese
 - **Microsoft Office:** Microsoft Word, Excel, Powerpoint

Instrumental Experience

- Rigaku Smartlab Diffractometer, Rigaku Miniflex Diffractometer, Empyrean Diffractometer
- ThermoScientific iCap 6000 Inductively Coupled Plasma-Optical Emission spectrometer
- JSM-6010Plus Scanning Electron Microscope instrument
- TA Q600 Thermogravimetric Analysis instrument, TA Q2000 Differential Scanning Calorimeter
- Quantachrome Nova 4200e Surface Area Instrument (BET)
- Maccor Cycle Life Tester, Bio-Logic, Four-Point Probe and CHI Potentiostat
- Pellet Press, 8000M Spex Mill, Dry Room, Glovebox