

Richard L. McNeel Associate Professor  
University of Nebraska-Lincoln, Department of Chemical and Biomolecular Engineering  
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## Education

- 09/2006–06/2009     **Dr.rer.nat. (Ph.D.)**  
Max Planck Institute for Solid State Research/University of Stuttgart,  
Stuttgart, Germany
- 06/2004–06/2006     **M.S. (*with distinction*), Quantum Chemistry**  
St. Petersburg State University, St. Petersburg, Russia
- 09/1999–06/2004     **Diploma (*with distinction*), Electrochemistry**  
St. Petersburg State University, St. Petersburg, Russia

## Professional Experience

- 07/2022–present     **Richard L. McNeel Associate Professor**  
07/2021–07/2022     **Associate Professor** (with tenure)  
08/2015–07/2021     **Assistant Professor**, Department of Chemical and Biomolecular Engineering, University of Nebraska–Lincoln
- 02/2012–08/2015     **Postdoctoral Research Associate**  
Pacific Northwest National Laboratory, Physical Sciences Division
- 10/2009–02/2012     **Postdoctoral Research Associate**  
University of California, Berkeley, Department of Materials Science and Engineering)  
University of California, Davis, Department of Chemical Engineering and Materials Science

## Awarded Research Grants

Total amount of funding generated by PI: ~\$1,400,000

### *Active Grants:*

2021	Collaborative Research with the Global Institute for Materials Research at Tohoku University, Japan, Awarded Amount: 380,000 JPY
07/2020–06/2025	<b>NSF CAREER</b> <i>"Advancing Mechanistic Understanding of Nanocrystal Dissolution in Aqueous Environments"</i> (single PI), Awarded Amount: \$520,244
07/2021	Supplement <b>NSF-INTERN</b> , Awarded Amount: \$35,924
09/2019–08/2022	<b>NSF CBET</b> <i>"Corrosion and Passivation Mechanisms of Li-Ion Battery Cathodes from Ab Initio Interfacial Reaction Dynamics"</i> (single PI), Awarded Amount: \$302,291
09/2018–08/2021	<b>American Chemical Society Petroleum Research Fund</b> <i>"Towards Atomistic Understanding of CO<sub>2</sub> Reduction to Fuels over Carbon-Based Metal-Free Electrocatalysts"</i> (single PI), Awarded Amount: \$110,000
2019–2021	<b>Nebraska Center for Energy Sciences Research</b> <i>"Conversion of Carbon Dioxide to Oxygenates by Plasma Catalysis"</i> (co-PI), Awarded Amount: \$63,710
2018–2021	<b>NSF-MRSEC</b> <i>"Understanding Electronic, Transport and Defect Properties of Low-Dimensional Ferroelectric Systems from First-Principles"</i> (co-PI), Awarded Amount: \$64,000
2016–present	National Energy Research Scientific Computing Center (NERSC)
2016–present	Extreme Science and Engineering Discovery Environment (XSEDE)

### *Completed Grants:*

2017–2018	<b>Nebraska EPSCoR FIRST Award</b> (single PI), Awarded Amount: \$25,000
2017–2018	<b>Nebraska Center for Energy Sciences Research Grant</b> <i>"Storing Renewable Energy for Nebraska and Beyond Using Vanadium Flow Batteries"</i> (co-PI), Awarded Amount: \$10,000
2017–2018	<b>UNL Interdisciplinary Research Grant</b> (co-PI), Awarded Amount: \$10,000
2015–2017	<b>NSF-MRSEC Seed Grant</b> <i>"Understanding Electronic, Transport and Defect Properties of Low-Dimensional Ferroelectric Systems from First-Principles"</i> (single PI), Awarded Amount: \$100,500
2015–2016	<b>Layman Award</b> from the University of Nebraska Foundation <i>"Rational Design of Electrolytes for Next-Generation Vanadium Redox Flow Batteries from First-Principles Modeling"</i> (single PI), Awarded Amount: \$10,000

## Awards and Fellowships

2019	NSF CAREER Award
2018	ACS PRF Award
2010	Travel Award to $\Psi_k$ -Workshop, Berlin, Germany
2009	Travel Award to Theoretical Spectroscopy School, ETH Zurich, Switzerland
2006–2009	Doctoral Fellowship of Max Planck Society (International Max Planck Research School for Advanced Materials)
2005	Fellowship to attend the 55th Meeting of Nobel Laureates in Lindau
2004	Personal Grant of St. Petersburg Government for Young Scientists

## Peer-Reviewed Research Publications (\* = Corresponding author)

### *Papers with V. Alexandrov as Principal Investigator*

59. Sharma S., Zagalskaya A., Weitzner S.E., Eggart L., Cho S., Hsu T., Chen X., Varley J.B., Alexandrov V., Orme C.A., Pham T.A. and Wood B.\* "Metal dissolution from first principles: potential-dependent kinetics and charge transfer," *Electrochimica Acta* (submitted)
58. Lamprecht X., Evazzade I., Ungerer I., Hromadko L., Macak J.M., Bandarenka A.\* and Alexandrov V.\* "Mechanisms of degradation of  $\text{Na}_2\text{Ni}[\text{Fe}(\text{CN})_6]$  functional electrodes in aqueous media: a combined theoretical and experimental study," *Chemistry of Materials* (submitted)
57. Nouri M., Kluge R.M., Haid R.W., Fortmann J., Ludwig A., Bandarenka A.\* and Alexandrov V.\* "Quantum electron tunneling at electrocatalytic interfaces," *ACS Catalysis* (under review)
56. Kim K., Zagalskaya A., Ng J.L., Hong J., Alexandrov V., Pham T.A., Su X.\* "Electrochemically-mediated reactive separation of nitrate to ammonia through multifunctional redox-electrodes," *Nature Energy* (under review)
55. Evazzade I., Zagalskaya A. and Alexandrov V.\* "On the role of interfacial water dynamics for electrochemical stability of  $\text{RuO}_2$  and  $\text{IrO}_2$ ," *ChemCatChem* (under revision)
54. Taji Y., Zagalskaya A., Evazzade I., Watzele S., Xue S., Schott C., Garlyyev B., Alexandrov V.\*, Gubanova E.\* and Bandarenka A.\* "Alkali metal cations change the hydrogen evolution reaction mechanisms at Pt electrodes in alkaline media," *Nano Materials Science* (under revision)
53. Gubanova E.\*, Schmidt T.O., Watzele S., Alexandrov V.\* and Bandarenka A.\* "Structure-dependent electrical double-layer capacitances of the basal plane  $\text{Pd}(hkl)$  electrodes in  $\text{HClO}_4$ ," *Journal of Physical Chemistry C* 126, 11414-11420 (2022)
52. Chatterjee S., Zamani E., Farzin S., Evazzade I., Obewhere O., Johnson T., Alexandrov V. and Dishari S.\* "Molecular-level control over ionic conduction and ionic current direction by designing macrocycle-based ionomers," *JACS Au* 2, 1144-1159 (2022)

51. Evazzade I., Zagalskaya A., and Alexandrov V.\* "Revealing elusive intermediates of platinum cathodic corrosion through DFT simulations," *Journal of Physical Chemistry Letters* 13, 3047-3052 (2022)
50. Czioska S., Boubnov A.\*, Escalera-Lopez D., Geppert J., Zagalskaya A., Rose P., Saraci E., Alexandrov V., Krewer U., Cherevko S.\*, and Grunwaldt J.-D.\* "Increased Ir-Ir interaction in iridium oxide during the oxygen evolution reaction at high potentials probed by operando spectroscopy," *ACS Catalysis* 11, 10043-10057 (2021)
49. Zagalskaya A., Evazzade I. and Alexandrov V.\* "Ab initio thermodynamics and kinetics of the lattice oxygen evolution reaction in iridium oxides," *ACS Energy Letters* 6, 1124-1133 (2021)
48. Speck F., Zagalskaya A., Alexandrov V. and Cherevko S.\* "Periodicity in the electrochemical dissolution of transition metals," *Angewandte Chemie International Edition* 60, 13343-13349 (2021)
47. Ryzhkov N.V., Ledovich O., Eggert L., Bund A., Paszuk A., Hannappel T., Klyukin K., Alexandrov V. and Skorb E.V.\* "Layer-by-layer polyelectrolyte assembly for the protection of GaP surface from photocorrosion," *ACS Applied Nano Materials* 4, 425-431 (2021)
46. Jiang Z. and Alexandrov V.\* "Electrocatalytic activity of oxygen-functionalized carbon electrodes for vanadium redox flow batteries from free-energy calculations," *ACS Applied Energy Materials* 3, 7543-7549 (2020)
45. Zhang Y., Yang Q., Tao L.L., Tsymbal E.Y., and Alexandrov V.\* "Effects of strain and film thickness on the stability of the rhombohedral phase of HfO<sub>2</sub>," *Physical Review Applied* 14, 014068 (2020)
44. Zagalskaya A. and Alexandrov V.\* "Mechanistic study of IrO<sub>2</sub> dissolution during electrocatalytic oxygen evolution reaction," *Journal of Physical Chemistry Letters* 11, 2695-2700 (2020)
43. Zagalskaya A. and Alexandrov V.\* "Role of defects in the interplay between adsorbate evolving and lattice oxygen mechanisms of oxygen evolution reaction in RuO<sub>2</sub> and IrO<sub>2</sub>," *ACS Catalysis* 10, 3650-3657 (2020)
42. Klyukin K. and Alexandrov V.\* "Kinetics of pH-dependent interactions between PD-1 and PD-L1 immune checkpoint proteins from molecular dynamics," *Proteins: Structure, Function, and Bioinformatics* 88(9), 1162-1168 (2020)
41. Jiang Z. and Alexandrov V.\* "Enhancing oxygen electroreduction activity of single-site Fe–N–C catalysts by a metal support," *Journal of Physical Chemistry C* 123, 30335-30340 (2019)
40. Yang Q.\*, Tao L., Zhang Y., Li M., Jiang Z., Tsymbal Y.,\* and Alexandrov V.\* "Ferroelectric tunnel junctions enhanced by a polar oxide barrier layer," *Nano Letters* 19, 7385-7393 (2019)

39. Yang Q., Tao L., Jiang Z., Zhou Y., Tsymbal Y.\*, and Alexandrov V.\* "Magnetoelectric effect at the Ni/HfO<sub>2</sub> interface induced by ferroelectric polarization," *Physical Review Applied* 12, 024044-024050 (2019)
38. Klyukin K., Zagalskaya A., and Alexandrov V.\* "Role of dissolution intermediates in promoting oxygen evolution reaction at RuO<sub>2</sub>(110) surface," *Journal of Physical Chemistry C* 123, 22151-22157 (2019) – Cover Page
37. Intan N., Klyukin K., and Alexandrov V.\* "Ab initio modeling of transition metal dissolution from LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> cathode," *ACS Applied Materials and Interfaces* 11, 20110-20116 (2019)
36. Jiang Z., Klyukin K., Miller K., and Alexandrov V.\* "Mechanistic theoretical investigation of self-discharge reactions in a vanadium redox flow battery," *Journal of Physical Chemistry B* 123, 3976-3983 (2019)
35. Klyukin K., Zagalskaya A., and Alexandrov V.\* "Ab initio thermodynamics of iridium surface oxidation and oxygen evolution reaction," *Journal of Physical Chemistry C* 122, 29350-29358 (2018)
34. Klyukin K., Tao L. L., Tsymbal E. Y.\*, and Alexandrov V.\* "Defect-assisted tunneling electroresistance in ferroelectric tunnel junctions," *Physical Review Letters* 121, 056601-056606 (2018) – Cover Page
33. Klyukin K., Rosso K. M., and Alexandrov V.\* "Iron dissolution from goethite ( $\alpha$ -FeOOH) surfaces in water by ab initio enhanced free energy simulations," *Journal of Physical Chemistry C* 122, 16086-16091 (2018)
32. Jiang Z., Klyukin K., and Alexandrov V.\* "Ab initio metadynamics study of VO<sub>2</sub><sup>+</sup>/VO<sup>2+</sup> redox reaction mechanism at the graphite edge-water interface," *ACS Applied Materials and Interfaces* 10, 20621-20626 (2018)
31. Intan N., Klyukin K., and Alexandrov V.\* "Theoretical insights into oxidation state of transition metals at (001) and (111) LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> spinel surfaces," *Journal of the Electrochemical Society* 165, A1099-A1103 (2018)
30. Ahn S., Klyukin K., Wakeham R.J., Lewis A.R., Alexander S., Carla F., Alexandrov V., and Andreoli E.\* "Poly-amide modified copper foam electrodes for enhanced electrochemical reduction of carbon dioxide," *ACS Catalysis* 8, 4132-4142 (2018)
29. Lu H., Lee D., Klyukin K., Tao L.L., Wang B., Lee H., Paudel T.R., Chen L.-Q., Tsymbal E.Y., Alexandrov V.\*, Eom C.-B.\*, and Gruverman A.\* "Tunneling hot spots in ferroelectric SrTiO<sub>3</sub>", *Nano Letters* 18, 491-497 (2018)
28. Intan N., Klyukin K., Zimudzi T., Hickner M., and Alexandrov V.\* "A combined theoretical-experimental study of interactions between vanadium ions and Nafion membrane in all-vanadium redox flow batteries", *Journal of Power Sources* 373, 150-160 (2018)

27. Jiang Z., Klyukin K., and Alexandrov V.\* "First-principles study of adsorption-desorption kinetics of  $V^{2+}/V^{3+}$  redox couple on graphite in a vanadium redox flow battery", *Physical Chemistry Chemical Physics (Communication)* 19, 14897-14901 (2017) – 2017 Hot Paper
26. Klyukin K. and Alexandrov V.\* "CO<sub>2</sub> adsorption and reactivity on rutile TiO<sub>2</sub>(110) in water: an *ab initio* molecular dynamics study", *Journal of Physical Chemistry C* 121, 10476-10483 (2017)
25. Klyukin K. and Alexandrov V.\* "Effect of intrinsic point defects on ferroelectric polarization behavior of SrTiO<sub>3</sub>", *Physical Review B* 95, 035301 (2017)
24. Alexandrov V.\*, Sushko M., Schreiber D., Bruemmer S., and Rosso K. "Adsorption and diffusion of atomic oxygen and sulfur at pristine and doped Ni surfaces with implications for stress corrosion cracking", *Corrosion Science* 113, 26-30 (2016)
23. Jiang Z., Klyukin K., and Alexandrov V.\* "Structure, hydrolysis, and diffusion of aqueous vanadium ions from Car-Parrinello molecular dynamics simulations", *Journal of Chemical Physics* 145, 114303-114311 (2016) – Editors' Choice
22. Sushko M.\*, Alexandrov V., Schreiber D., Rosso K., and Bruemmer S. "Multiscale model of metal alloy oxidation at grain boundaries", *Journal of Chemical Physics* 142, 214114-214121 (2015)

*Papers from V. Alexandrov's Postdoctoral and Doctoral Work*

21. Alexandrov V.\* and Rosso K. "Ab initio modeling of Fe(II) adsorption and interfacial electron transfer at goethite ( $\alpha$ -FeOOH) surfaces", *Physical Chemistry Chemical Physics* 17, 14518-14531 (2015)
20. Alexandrov V.\*, Sushko M., Schreiber D., Bruemmer S., and Rosso K. "Ab initio modeling of bulk and intragranular diffusion in Ni alloys", *Journal of Physical Chemistry Letters* 6, 1618-1623 (2015)
19. Solomon J. M.\*, Alexandrov V., Sadigh B., Navrotsky A., and Asta M. "Computational study of the energetics and defect-clustering tendencies for Y and La-doped UO<sub>2</sub>", *Acta Materialia* 78, 282-289 (2014)
18. Alexandrov V.\* and Rosso K. "Electron transport in pure and substituted iron oxyhydroxides by small polaron migration", *Journal of Chemical Physics* 140, 234701-234709 (2014)
17. Alexandrov V.\*, Grønbech-Jensen N., Navrotsky A., and Asta M. "Theoretical study of mixing energetics in homovalent fluorite-structured oxide solid solutions", *Journal of Nuclear Materials* 444, 292-297 (2014)
16. Alexandrov V.\* and Rosso K. "Insights into the mechanism of Fe(II) adsorption and oxidation at Fe-clay mineral surfaces from first-principles calculations", *Journal of Physical Chemistry C* 117, 22880-22886 (2013)

15. Alexandrov V.\*, Neumann A., Scherer M., and Rosso K. "Electron exchange and conduction in nontronite from first-principles", *Journal of Physical Chemistry C* 117(5), 2032-2040 (2013)
14. Alexandrov V., Shvareva T. Y., Hayun S., Asta M., and Navrotsky A.\* "Actinide dioxides in water: interactions at the interface", *Journal of Physical Chemistry Letters* 2, 3130-3134 (2011)
13. Shvareva T. Y., Alexandrov V., Asta M., and Navrotsky A.\* "Energetics of mixing in ThO<sub>2</sub>-CeO<sub>2</sub> fluorite solid solutions", *Journal of Nuclear Materials* 419, 72-75 (2011)
12. Alexandrov V., Piskunov S.\*, Zhukovskii Yu., Kotomin E., and Maier J. "First-principles modeling of oxygen interaction with SrTiO<sub>3</sub> (001) surface: comparative density-functional LCAO and plane-wave study", *Integrated Ferroelectrics* 123, 10-17 (2011)
11. Kotomin E.\*, Alexandrov V., Gryaznov D., Evarestov R.A., and Maier J. "Confinement effects for ionic carriers in SrTiO<sub>3</sub> ultrathin films: first-principles calculations of oxygen vacancies", *Physical Chemistry Chemical Physics (Communication)* 13, 923 (2011)
10. Alexandrov V., Grønbech-Jensen N., Navrotsky A., and Asta M.\* "First-principles computational study of defect clustering in solid solutions of ThO<sub>2</sub> with trivalent oxides", *Physical Review B* 82, 174115 (2010)
9. Alexandrov V.\*, Kotomin E.A., Maier J., and Evarestov R.A. "First-principles study of bulk and surface oxygen vacancies in SrTiO<sub>3</sub> crystal", *European Physical Journal B* 72, 53-57 (2009)
8. Alexandrov V.\*, Kotomin E.A., Maier J., and Evarestov R.A. "Ab initio modeling of spin and charge ordering and lattice dynamics in CaFeO<sub>3</sub> crystals", *Journal of Chemical Physics* 129, 214704 (2008)
7. Alexandrov V.\*, Maier J., and Evarestov R.A. "Ab initio study of SrFe<sub>x</sub>Ti<sub>1-x</sub>O<sub>3</sub>: Jahn-Teller distortion and electronic structure", *Physical Review B* 77, 075111 (2008)
6. Alexandrov V.\* Evarestov R.A., Kotomin E.A., and Maier J. "Ab initio study of bulk and surface iron defects in SrTiO<sub>3</sub>", *Journal of Physics: Conference Series* 72, 53 (2008)
5. Evarestov R.A., Bandura A.V.\*, and Alexandrov V. "Adsorption of water on (001) surface of SrTiO<sub>3</sub> and SrZrO<sub>3</sub> cubic perovskites: hybrid HF-DFT LCAO calculations", *Surface Science* 72, 1844 (2007)
4. Evarestov R.A.\*, Bandura A.V., and Alexandrov V. "Hybrid HF-DFT comparative study of SrZrO<sub>3</sub> and SrTiO<sub>3</sub> (001) surface properties", *Physica Status Solidi (b)* 243, 2756 (2006)
3. Evarestov R.A.\*, Tupitsyn I.I., Bandura A.V., and Alexandrov V. "Ab initio calculations and analysis of chemical bonding in SrTiO<sub>3</sub> and SrZrO<sub>3</sub> cubic crystals", *International Journal of Quantum Chemistry* 106, 2191 (2006)

2. Evarestov R.A.\*, Bandura A.V., and Alexandrov V. "Calculations of the electronic structure of crystalline  $\text{SrZrO}_3$  in the framework of the density-functional theory in the LCAO approximation", *Physics of the Solid State* 47 (12), 2248 (2005)
1. Evarestov R.A.\*, Bandura A.V., Alexandrov V. and Kotomin E.A. "DFT LCAO and plane wave calculations of  $\text{SrZrO}_3$ ", *Physica Status Solidi (Rapid Research Letters)* 242 (2), R11 (2005)

## Technical Presentations by V. Alexandrov

(I–Invited; C–Contributed; P–Poster)

02/2022	Institute of Physical Chemistry, Justus Liebig University Giessen, Germany, " <i>Atomic-Scale Coupling between Activity and Stability of Water-Splitting Electrocatalysts</i> " (I)
02/2022	Physics Department, Technical University of Munich, Germany, " <i>Atomic-Scale Coupling between Activity and Stability of Water-Splitting Electrocatalysts</i> " (I)
01/2022	Schloss Ringberg Conference Site of the Max Planck Society, Germany, " <i>Atomic-Scale Coupling between Electrocatalytic Activity and Electrode Corrosion</i> " (I, webinar)
12/2021	MRS Fall Meeting, " <i>Lattice Oxygen Evolution Reaction and Its Role in Electrochemical Stability of Iridium Oxides</i> " (C, webinar)
08/2020	NSF CBET 2020 Energy Storage Workshop, " <i>Computational Insights into Interfacial Chemistry of Redox-Flow and Lithium-Ion Batteries</i> " (I, webinar)
07/2020	Lawrence Livermore National Laboratory, Quantum Simulations Group, " <i>Computational Insights into the Interplay between Stability and Activity of Water Splitting Electrocatalysts</i> " (I, webinar)
12/2019	MRS Fall Meeting, Boston, MA, " <i>Transition Metal Dissolution from <math>\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4</math> Cathode Investigated by Ab Initio Free Energy Simulations</i> " (C)
08/2019	ACS Fall Meeting, San Diego, CA, " <i>Theoretical Insights into Activity-Stability Relationships of Transition Metal Based Electrocatalysts</i> " (I)
07/2019	Computational Materials Chemistry Workshop, Telluride, CO, " <i>Solution and Interfacial Electrochemistry of All-Vanadium Redox Flow Batteries from First-Principles</i> " (I)
03/2019	Nebraska NSF-MRSEC Review, Lincoln, NE, " <i>Defect-Assisted Tunneling Electroresistance in Ferroelectric Tunnel Junctions</i> " (I)
02/2019	Gordon Research Conference " <i>Chemical Reactions at Surfaces</i> ", Ventura, CA, (P)



- 11/2018 American Association for Cancer Research Meeting: Tumor Immunology and Immunotherapy, Miami Beach, FL, "*Molecular Dynamics Study of pH-Dependent Interactions between Immune Checkpoint Receptor PD-1 and Its Ligand PD-L1*" (P)
- 10/2018 ACS Midwest Regional Meeting, Ames, IA, "*First-Principles Molecular Dynamics Studies of Catalytic CO<sub>2</sub> Conversion Reactions in Aqueous Solutions*" (I)
- 05/2018 ITMO University, Department of Chemistry and Molecular Biology, St. Petersburg, Russia, "*Many Faces of Electrochemical Interfaces: Examples from Solid State and Redox Flow Batteries*" (I)
- 02/2018 Gordon Research Conference, Ventura, CA, "*Batteries*" (P)
- 02/2017 Gordon Research Conference, Ventura, CA, "*Nanomaterials for Applications in Energy Technology*" (P)
- 10/2016 University of Iowa, Department of Chemistry, "*Application of First-Principles Simulations to Explore Physical/Chemical Phenomena for Sustainable Energy Applications*" (I)
- 03/2016 ACS Spring Meeting, San Diego, CA, "*First-Principles Investigation of Fe(II) Adsorption and Electron Transfer at the Goethite/Water Interfaces*" (C)
- 02/2015 University of Nebraska-Lincoln, Dept. of Chemical and Biomolecular Engineering, Lincoln, NE, "*Understanding Defect Behavior in Advanced Materials through Ab Initio Based Multiscale Modeling*" (I)
- 04/2014 University of California, Los Angeles, Dept. of Civil and Environmental Engineering, Los Angeles, CA, "*Understanding Defect Behavior in Advanced Materials through Ab Initio Based Multiscale Modeling*" (I)
- 03/2013 ACS Spring Meeting, Dallas, TX, "*Fe(II) Adsorption and Electron Exchange with Fe(III) at FeOOH (Goethite) Surfaces*" (C)
- 08/2012 Biogeochemistry and Redox Transformations of Iron (biennial workshop), Telluride, CO, "*Computational Modeling of Fe-Bearing Redox-Active Mineral Systems*" (I)
- 10/2011 Pacific Northwest National Laboratory, Physical Sciences Division, Richland, WA, "*Computational Study of Actinide-Oxide Fluorite-Structured Compounds*" (I)
- 11/2011 MRS Fall Meeting, Boston, MA, "*Computational Modeling of Iso- and Aliovalently Doped ThO<sub>2</sub> and UO<sub>2</sub>*" (C)
- 10/2011 Materials Science and Technology Meeting, Columbus, OH, "*Computational Study of Defect Clustering and Diffusion in Solid Solutions of Aliovalently Doped ThO<sub>2</sub>*" (C)
- 06/2011 Energy Frontier Research Center "Materials Science of Actinides" Science Review Meeting, Notre Dame, IN, "*Water Adsorption on Surfaces of Fluorite-Structured ThO<sub>2</sub> and CeO<sub>2</sub>: First-Principles Computational Studies*" (I)
- 03/2011 ACS Spring Meeting, Anaheim, CA, "*First-Principles Study of Surface Stability and Water Adsorption on ThO<sub>2</sub> Surfaces*" (C)

03/2010 APS Spring Meeting, Portland, OR, *"First-Principles Modeling of ThO<sub>2</sub> Solid Solutions with Oxides of Trivalent Cations"* (C)

## Teaching Experience

CHME 312 Chemical Engineering Computation	Spring, Fall 2016, Fall 2017, 2019, 2020, 2021, 2022
CHME 412/812 Introduction to Atomistic Simulations	Spring 2017, 2018, 2019
CHME 442 Chemical Reactor Engineering and Design	Spring 2021

## Researchers Supervised

Name	Title	Period	Position
Payal Chaudhary	PhD student	08/2021 - current	
Mohammad Nouri	PhD student	08/2021 - current	
Iman Evazzade	Postdoc	06/2019 - current	
Alexandra Zagalskaya	PhD student	07/2018 - 07/2022	Lawrence Livermore Nat Lab
Jae Hyun Lim	High-school student	05/2017 - 08/2017	Harvard
Kaellen Miller	Undergraduate student	08/2016 - 12/2016	UNL
Nadia Intan	PhD student	07/2016 - 11/2019	University of Washington
Zhen Jiang (Jason)	PhD student	01/2016 - 07/2019	University of Pennsylvania
Konstantin Klyukin	Postdoc	02/2016 - 02/2019	Assistant Professor at Auburn
Qiong Yang	Visiting Scholar	10/2018 - 03/2020	Professor in China

## Awards to Supervised Researchers

Payal Chaudhary	Othmer Fellowship of the College of Engineering at UNL (2021)
Nadia Intan	1st place in poster session at the Supercomputer and Life Science Symposium at UNL (2019)
Nadia Intan	Chemical Engineering Student Support Fund Fellowship, UNL (2019)
Nadia Intan	Milton E. Mohr Award of the College of Engineering, UNL (2018)
Nadia Intan	NSF funding to attend CECAM School on Computational Materials Science, Lausanne, Switzerland (July 2017)
Zhen Jiang	NSF funding to attend CECAM School on Computational Materials Science, Lausanne, Switzerland (July 2017)
Qiong Yang	China Government Council Scholarship to visit UNL (2018-2019)

## Professional Service

2021	MRS Spring Meeting, Seattle, Symposium Organizer "Advances in Conversion Electrodes for Reliable Electrochemical Energy Storage"
2016	ACS Meeting, Philadelphia, Session Organizer "Molecular Modeling of Surface-Mediated Electrochemical and Sorption Reactions at Environmental Interfaces"
2015-present	Reviewer for DOE, NSF, DOD
2018-present	Reviewer for ACS PRF
2009-present	Manuscript reviewer for Chemical Reviews, Nature Communications, Nature Catalysis, ACS Catalysis, Applied Catalysis B, Advanced Materials, Journal of Physical Chemistry, Chemistry of Materials, Journal of Chemical Physics, Journal of Power Sources, Journal of Materials Chemistry, Scientific Reports, Surface Science, Acta Materialia, Computational Materials Science, Inorganic Chemistry, Electrochimica Acta