

Vitaly Alexandrov

Richard L. McNeel Associate Professor

Department of Chemical and Biomolecular Engineering, University of Nebraska-Lincoln

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EDUCATION

Dr.rer.nat. (Ph.D.), Computational Chemistry, Adviser: Joachim Maier

Max Planck Institute for Solid State Research/University of Stuttgart, Germany, 2006-2009

M.S., Quantum Chemistry (*with distinction*), Adviser: Robert Evarestov

St. Petersburg State University, St. Petersburg, Russia, 2004-2006

Diploma, Chemistry (*with distinction*), specialization in electrochemistry, Adviser: Valery Malev

St. Petersburg State University, St. Petersburg, Russia, 1999-2004

RESEARCH EXPERIENCE

Richard L. McNeel Associate Professor, University of Nebraska-Lincoln, 2022 – present

Visiting Professor, Tohoku University, Institute for Materials Research, Japan, 2023

Visiting Professor (sabbatical), Technical University of Munich, Germany, 2022

Associate Professor (with tenure), University of Nebraska-Lincoln, 2021 – 2022

Assistant Professor, Chemical and Biomolecular Engineering, University of Nebraska-Lincoln, 2015 – 2021

Postdoctoral Scholar, Pacific Northwest National Laboratory, USA, 2012 – 2015, Adviser: Kevin Rosso

Postdoctoral Scholar, UC Davis/UC Berkeley, USA 2009-2012, Adviser: Mark Asta

TEACHING EXPERIENCE

Instructor. University of Nebraska-Lincoln, Chemical and Biomolecular Engineering, 2015-present

- CHME 212 Chemical Engineering Computation I
- CHME 312 Chemical Engineering Computation II
- CHME 412/812 Introduction to Atomistic Simulations
- CHME 442 Chemical Reactor Engineering and Design
- CHME 486/886 Electrochemical Engineering

HONORS AND AWARDS

- National Science Foundation CAREER Award, 2020
- American Chemical Society Petroleum Research Fund Award, 2018
- Layman Award, UNL, 2015
- Doctoral Fellowship of Max Planck Society (International Max Planck Research School for Advanced Materials), 2006-2009
- Fellowship to attend the 55th Meeting of Nobel Laureates, Lindau, Germany, 2005
- Personal Grant of St. Petersburg Government for Young Scientists, 2004

PROFESSIONAL SERVICE

- Member of the Journal of Physical Chemistry C Editorial Advisory Board (Jan 2024 – Dec 2026)
- Chair of the session “*Design and Synthesis of Metal and Bimetallic Single-Atom Catalysts*”, 28th North American Meeting (NAM) of the North American Catalysis Society, Providence, 2023
- Co-organizer, symposium “*Advances in Conversion Electrodes for Reliable Electrochemical Energy Storage*,” MRS Spring Meeting, Seattle, 2021
- Co-organizer, session “*Molecular Modeling of Surface-Mediated Electrochemical and Sorption Reactions at Environmental Interfaces*,” ACS Fall Meeting, Philadelphia, 2016.

REVIEW PANELS

Ad hoc reviewer for journals:

ACS Catalysis, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Chemistry of Materials, Chemical Reviews, Nature Communications, Nature Catalysis, Applied Catalysis B, Journal of Chemical Physics, Physical Chemistry Chemical Physics, Advanced Materials, Angewandte Chemie, ChemCatChem, Electrochimica Acta, Inorganic Chemistry, Physical Review B

Ad hoc proposal reviewer: DOE, DOD, NSF, American Chemical Society Petroleum Research Fund, DFG (German Research Foundation)

Review Panels: NSF.

PROFESSIONAL MEMBERSHIPS

- American Chemical Society, American Institute of Chemical Engineers

RESEARCH FUNDING

Total amount of funding generated by the PI is ~\$1.3M.

11. **NSF CAREER** Award “*Advancing mechanistic understanding of nanocrystal dissolution in aqueous environments*” (single PI), 2020-2025. Awarded Amount: \$520,244.

10. **NSF-INTERN** Supplement (single PI), 2021. Awarded Amount: \$35,924.

9. **NSF CBET** “*Corrosion and passivation mechanisms of Li-ion battery cathodes from ab initio interfacial reaction dynamics*” (single PI), 2019-2024. Awarded Amount: \$302,291.

8. **ACS Petroleum Research Fund** “Towards atomistic understanding of CO₂ reduction to fuels over carbon-based metal-free catalysts” (single PI), 2018-2021. Awarded Amount: \$110,000.

7. **Nebraska Center for Energy Sciences Research** grant “*Conversion of carbon dioxide to oxygenates by plasma catalysis*” (co-PI), 2019-2021. Awarded Amount: \$63,710.

6. **NSF-MRSEC** “*Understanding of electronic, transport, and defect properties of low-dimensional ferroelectric systems from first-principles*” (co-PI), 2018-2021. Awarded Amount: \$64,000.

5. **Nebraska EPSCoR FIRST** Award (single PI), 2017-2018. Awarded Amount: \$25,000.
4. **Nebraska Center for Energy Sciences Research** grant “*Storing renewable energy for Nebraska and beyond using vanadium flow batteries*” (co-PI), 2017-2018. Awarded Amount: \$10,000.
3. **UNL Interdisciplinary Research** grant (co-PI), 2017-2018. Awarded Amount: \$10,000.
2. **NSF-MRSEC** Seed Grant “*Understanding of electronic, transport, and defect properties of low-dimensional ferroelectric systems from first-principles,*” (single PI), 2015-2017. Awarded Amount: \$100,500.
1. **Layman Award** from the University of Nebraska Foundation “*Rational design of electrolytes for next-generation of vanadium redox flow batteries from first-principles modeling,*” (single PI), 2015-2016. Awarded Amount: \$10,000.

PUBLICATIONS (* corresponding author)

66. Schott C.M., Song K.-T., Yu H., Goetz R., Haimerl F., Schneider P.T., Zhang Q., Schmidt T.O., Gubanov E., Alexandrov V.*, and Bandarenka A.S.* "How to assess and predict electrical double layer properties. Implications for electrocatalysis," *Chemical Reviews* (submitted).
65. Xue S., Chaudhary P., Nouri M.R., Gubanov E., Garlyyev B., Alexandrov V.*, and Bandarenka A.S.* "Impact of Pt electrode surface structure on the electrical double layer capacitance," *Journal of the American Chemical Society* (under revision).
64. Song K.-T., Zagalskaya A., Schott C.M., Schneider P.M., Garlyyev B., Alexandrov V., and Bandarenka A.S.* "Influence of alkali metal cations on the oxygen reduction reaction activity of Pt₅Y and Pt₅Gd alloys," *Angewandte Chemie International Edition* (submitted).
63. Chaudhary P., Zagalskaya A., Over H., and Alexandrov V.* "Strain-dependent activity-stability relations in RuO₂ and IrO₂ oxygen evolution catalysts," *ChemElectroChem* (submitted).
62. Zagalskaya A., Nouri M.R., and Alexandrov V.* "Mechanistic understanding of electrode corrosion driven by water electrolysis," *Current Opinion in Electrochemistry* 41, 101352 (2023) – an invited Review article.
61. Zagalskaya A., Chaudhary P., and Alexandrov V.* "Corrosion of electrochemical energy materials: Stability analyses beyond Pourbaix diagrams," *Journal of Physical Chemistry C* 127, 14587-14598 (2023) – an invited Perspective article (Cover Page).
60. Chaudhary P., Evazzade I., Belosludov R. and Alexandrov V.* "Computational discovery of active and selective metal-nitrogen-graphene catalysts for electrooxidation of water to H₂O₂," *ChemCatChem* e202300055 (2023).
59. Nouri M., Kluge R.M., Haid R.W., Fortmann J., Ludwig A., Bandarenka A.* and Alexandrov V.* "Electron tunneling at electrocatalytic interfaces," *Journal of Physical Chemistry C* 127, 6321-6327 (2023).
58. Kim K., Zagalskaya A., Ng J.L., Hong J., Alexandrov V., Pham T.A., Su X.* "Coupling nitrate capture with ammonia production through bifunctional redox-electrodes," *Nature*

Communications 14, 823 (2023).

57. 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," *Journal of Physical Chemistry C* 127, 2204-2214 (2023).

56. 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* (in press).

55. 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* 437, 141443 (2023).

54. Evazzade I., Zagalskaya A. and Alexandrov V.* "On the role of interfacial water dynamics for electrochemical stability of RuO_2 and IrO_2 ," *ChemCatChem* e202200932 (2022).

53. Gubanova E.*, Schmidt T.O., Watzele S., Alexandrov V.* and Bandarenka A.* "Structure-dependent electrical double-layer capacitances of the basal plane Pd(*hkl*) electrodes in 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., Tsybmal E.Y., and Alexandrov V.* "Effects of strain and film thickness on the stability of the rhombohedral phase of HfO_2 ," *Physical Review Applied* 14, 014068 (2020).

44. Zagalskaya A. and Alexandrov V.* "Mechanistic study of IrO₂ 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 RuO₂ and IrO₂," *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/HfO₂ 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 RuO₂(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_{0.5}Mn_{1.5}O₄ 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 (α -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⁺/VO²⁺ 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_{0.5}Mn_{1.5}O₄ 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., Tsybal E.Y., Alexandrov V.*, Eom C.-B.*, and Gruverman A.* "Tunneling hot spots in ferroelectric SrTiO₃", *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 V²⁺/V³⁺ redox couple on graphite in a vanadium redox flow battery", *Physical Chemistry Chemical Physics (Communication)* 19, 14897-14901 (2017) – Hot paper.
26. Klyukin K. and Alexandrov V.* "CO₂ adsorption and reactivity on rutile TiO₂(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 SrTiO₃", *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).
21. Alexandrov V.* and Rosso K. "Ab initio modeling of Fe(II) adsorption and interfacial electron transfer at goethite (α -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 UO₂", *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 ThO₂-CeO₂ 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 SrTiO₃ (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 SrTiO₃ 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 ThO₂ 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 SrTiO₃ 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 CaFeO₃ crystals", *Journal of Chemical Physics* 129, 214704 (2008).

7. Alexandrov V.*, Maier J., and Evarestov R.A. "Ab initio study of SrFe_xTi_{1-x}O₃: 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 SrTiO₃", *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 SrTiO₃ and SrZrO₃ 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 SrZrO₃ and SrTiO₃ (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 SrTiO₃ and SrZrO₃ 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 SrZrO₃ 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 SrZrO₃", *Physica Status Solidi (Rapid Research Letters)* 242 (2), R11 (2005).

PRESENTATIONS (I – invited, C – contributed, P – poster)

29. Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln, "Atomic-Scale Insights into Activity-Stability-Selectivity Properties of Water-Splitting Electrocatalysts" (I), 10/2022.

28. Institute of Physical Chemistry, Justus Liebig University Giessen, Germany, "Atomic-Scale Coupling between Activity and Stability of Water-Splitting Electrocatalysts" (I), 02/2022.

27. Physics Department, Technical University of Munich, Germany, "Atomic-Scale Coupling between Activity and Stability of Water-Splitting Electrocatalysts" (I), 02/2022.

26. Schloss Ringberg Conference Site of the Max Planck Society, Germany, "Atomic-Scale Coupling between Electrocatalytic Activity and Electrode Corrosion" (I, webinar), 01/2022.

25. MRS Fall Meeting, "Lattice Oxygen Evolution Reaction and Its Role in Electrochemical Stability of Iridium Oxides" (C, webinar), 12/2021.

24. NSF CBET 2020 Energy Storage Workshop, "Computational Insights into Interfacial Chemistry of Redox-Flow and Lithium-Ion Batteries" (I, webinar), 08/2020.

23. Lawrence Livermore National Laboratory, Quantum Simulations Group, "Computational Insights into the Interplay between Stability and Activity of Water Splitting Electrocatalysts" (I, webinar), 07/2020.

22. MRS Fall Meeting, Boston, MA, "Transition Metal Dissolution from LiNi_{0.5}Mn_{1.5}O₄ Cathode Investigated by Ab Initio Free Energy Simulations" (C), 12/2019.

21. ACS Fall Meeting, San Diego, CA, "Theoretical Insights into Activity- Stability Relationships of Transition Metal Based Electrocatalysts" (I), 08/2019.

20. Computational Materials Chemistry Workshop, Telluride, CO, "Solution and Interfacial Electrochemistry of All-Vanadium Redox Flow Batteries from First-Principles" (I), 07/2019.

19. Nebraska NSF-MRSEC Review, Lincoln, NE, "Defect-Assisted Tunneling Electroresistance in Ferroelectric Tunnel Junctions" (I), 03/2019.

18. Gordon Research Conference "Chemical Reactions at Surfaces", Ventura, CA, (P), 02/2019.

17. 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), 11/2018.

16. ACS Midwest Regional Meeting, Ames, IA, "First-Principles Molecular Dynamics Studies of Catalytic CO₂ Conversion Reactions in Aqueous Solutions" (I), 10/2018.

15. 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), 05/2018.
14. Gordon Research Conference, Ventura, CA, *"Batteries"* (P), 02/2018.
13. Gordon Research Conference, Ventura, CA, *"Nanomaterials for Applications in Energy Technology"* (P), 02/2017.
12. University of Iowa, Department of Chemistry, *"Application of First- Principles Simulations to Explore Physical/Chemical Phenomena for Sustainable Energy Applications"* (I), 10/2016.
11. ACS Spring Meeting, San Diego, CA, *"First-Principles Investigation of Fe(II) Adsorption and Electron Transfer at the Goethite/Water Interfaces"* (C), 03/2016.
10. 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), 02/2015.
9. 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), 04/2014.
8. ACS Spring Meeting, Dallas, TX, *"Fe(II) Adsorption and Electron Exchange with Fe(III) at FeOOH (Goethite) Surfaces"* (C), 03/2013.
7. Biogeochemistry and Redox Transformations of Iron (biennial workshop), Telluride, CO, *"Computational Modeling of Fe-Bearing Redox-Active Mineral Systems"* (I), 02/2012.
6. Pacific Northwest National Laboratory, Physical Sciences Division, Rich- land, WA, *"Computational Study of Actinide-Oxide Fluorite-Structured Compounds"* (I), 10/2011.
5. MRS Fall Meeting, Boston, MA, *"Computational Modeling of Iso- and Aliovalently Doped ThO₂ and UO₂"* (C), 11/2011.
4. Materials Science and Technology Meeting, Columbus, OH, *"Computational Study of Defect Clustering and Diffusion in Solid Solutions of Aliovalently Doped ThO₂"* (C), 10/2011.
3. Energy Frontier Research Center "Materials Science of Actinides" Science Review Meeting, Notre Dame, IN, *"Water Adsorption on Surfaces of Fluorite-Structured ThO₂ and CeO₂: First-Principles Computational Studies"* (I), 06/2011.
2. ACS Spring Meeting, Anaheim, CA, *"First-Principles Study of Surface Stability and Water Adsorption on ThO₂ Surfaces"* (C), 03/2011.
1. APS Spring Meeting, Portland, OR, *"First-Principles Modeling of ThO₂ Solid Solutions with Oxides of Trivalent Cations"* (C), 03/2010.

SUPERVISED RESEARCHERS

Name	Title	Period	Next Position
Payal Chaudhary	PhD student	08/2021 - current	
Mohammad Nouri	PhD student	08/2021 - current	
Iman Evazzade	Postdoc	06/2019 - 02/2023	BMW
Sofia Sarroub-Le Sueur	High-school student	06/2023 - 08/2023	Lincoln East High School
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
Akshat Saraf	Undergraduate student	05/2022 – 08/2022	University of Göttingen