

Konstantin Klyukin

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Materials Engineering
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PROFESSIONAL EXPERIENCE

- 2022–present **Assistant Professor**, Department of Mechanical Engineering, Materials Engineering Program, Auburn University, AL, USA
- 2019–2021 **Postdoctoral Associate**, Department of Materials Science and Engineering, Massachusetts Institute of Technology, MA, USA
References: Prof. Bilge Yildiz
- 2016–2019 **Postdoctoral Associate**, Department of Chemical and Biomolecular Engineering, University of Nebraska-Lincoln, NE, USA
References: Prof. Vitaly Alexandrov

EDUCATION

- 2012–2016 **Ph.D. in Condensed Matter Physics**, Saint Petersburg State University, Russia.
Advisor: Prof. Marina Shelyapina
- 2010–2012 **M.S. in Applied Mathematics and Physics**, Saint Petersburg State University, Russia.
- 2006–2010 **B.S. in Applied Mathematics and Physics**, Saint Petersburg State University, Russia.

RESEARCH INTERESTS

ab initio methods (density functional theory, molecular dynamics, high-throughput materials design); predictive data analytics models; defect chemistry; ion conductors; fuel cells; batteries; corrosion; heterogeneous catalysis; ferroelectrics; brain-inspired computing; hydrogen storage.

PUBLICATIONS

1. A. Kumar, **K. Klyukin**, S. Ning, C. Ozsoy-Keskinbora, M. Ovsyanko, F. van Uden, R. Krijnen, B. Yildiz, C. A. Ross and J. M. LeBeau, Antisite Defects Stabilized by Antiphase Boundaries in YFeO₃ Thin Films, *Advanced Functional Materials*, 2107017, 2021.
2. M. Huang, M. U. Hasan, **K. Klyukin**, J. Zehner, L. Caretta, K-Y. Lee, J. Chang, K. Leistner, B. Yildiz, and G. S. D. Beach. Voltage control of ferrimagnetic order and voltage-assisted writing of ferrimagnetic spin textures by solid-state hydrogen gating, *Nature Nanotechnology* 16 (9), 981-988, 2021.

3. S. Ning, A. Kumar, **K. Klyukin**, JH Kim, T. Su, HS Kim, JM. LeBeau, B. Yildiz and C. A. Ross, An antisite defect mechanism for room temperature ferroelectricity in orthoferrites, *Nature Communications*, 12:4298, 2021.
4. E. Cho, **K. Klyukin**, S. Ning, B. Yildiz, C.A. Ross, First-principles calculation of oxygen vacancy effects on the magnetic properties of the perovskite, *Physical Review Materials*, 2021, 5(9), 094413
5. JW Jung, JS Nam, **K. Klyukin**, DY Youn and Il-Doo Kim, Straightforward strategy toward a shape-deformable carbon-free cathode for flexible Li-air batteries in ambient air, *Nano Energy*, Nano Energy, 83, 105821, 2021.
6. **K. Klyukin**, G. Beach and B. Yildiz. Hydrogen tunes magnetic anisotropy by affecting local hybridization at the interface of a ferromagnet with nonmagnetic metals, *Physical Review Materials* 4 (10), 104416, 2020.
7. N. V. Ryzhkov, O. Ledovich, L. Eggert, A. Bund, A. Paszuk, T. Hannappel, **K. Klyukin**, V. Alexandrov and E. V. Skorb, Layer-by-Layer Polyelectrolyte Assembly for the Protection of GaP Surfaces from Photocorrosion, *ACS Applied Nano Materials*, 4(1), 425–431, 2020.
8. X. Yao, **K. Klyukin**, W. Lu, M. Onen, D. Kim, N. Emond, I. Waluyo, A. Hunt, J. A. del Alamo, Ju Li, and Bilge Yildiz. Protonic Solid-State Electrochemical Synapse for Analog Computing, *Nature Communications*, 11, 3134, 2020.
9. **K. Klyukin**, V. Alexandrov, Kinetics of pH-Dependent Interactions between PD-1 and PD-L1 Immune Checkpoint Proteins, *Proteins Structure Function and Bioinformatics*, 88(9), 1162-1168, 2020.
10. H. Mauroy, **K. Klyukin**, M.G. Shelyapina, D.A. Keen, A. Thøgersen, B.C. Hauback and M.H. Sørby. Short-range structure of $\text{Ti}_{0.63}\text{V}_{0.27}\text{Fe}_{0.1}\text{D}_{1.73}$ from neutron total scattering and Reverse Monte Carlo modeling, *Energies* 13(8), 1947, 1-14, 2020.
11. **K. Klyukin**, A. Zagalskaya, and V. Alexandrov, Role of Dissolution Intermediates in Promoting Oxygen Evolution Reaction at $\text{RuO}_2(110)$ Surface, *The Journal of Physical Chemistry C*, 123(36), 22151-22157, 2019. *Featured on the cover*
12. N. Intan, **K. Klyukin**, and V. Alexandrov. Ab Initio Modeling of Transition Metal Dissolution from $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ Cathode, *ACS Appl. Mater. Interfaces* 11, 20110-20116, 2019.
13. Z. Jiang, **K. Klyukin**, K. Miller, and V. Alexandrov. Mechanistic Theoretical Investigation of Self-Discharge Reactions in a Vanadium Redox Flow Battery. *Journal of Physical Chemistry B*, 123, 3976–3983, 2019.
14. **K. Klyukin**, A. Zagalskaya, and V. Alexandrov. Ab Initio Thermodynamics of Iridium Surface Oxidation and Oxygen Evolution Reaction, *The Journal of Physical Chemistry C*, 122 (51), 29350-29358, 2018.
15. **K. Klyukin**, K. M. Rosso, and V. Alexandrov. Iron Dissolution from Goethite ($\alpha\text{-FeOOH}$) Surfaces in Water by Ab Initio Enhanced Free-Energy Simulations. *The Journal of Physical Chemistry C*, 122(28):16086–16091, 2018.
16. Z. Jiang, **K. Klyukin**, and V. Alexandrov. Ab Initio Metadynamics Study of $\text{VO}_2^+/\text{VO}^{2+}$ Redox Reaction Mechanism at the Graphite Edge/Water Interface. *ACS Appl. Mater. Interfaces*, 10(24):20621–20626, 2018.
17. O.O. Bavrina, M. G. Shelyapina, **K. Klyukin**, D. Fruchart. First-principles modeling of hydrogen site solubility and diffusion in disordered Ti-V-Cr alloys. *International Journal of Hydrogen Energy*, 43(36):17338-17345, 2018.

18. **K. Klyukin**, LL Tao, E. Y. Tsymbal, and V. Alexandrov. Defect-Assisted Tunneling Electroresistance in Ferroelectric Tunnel Junctions. *Physical Review Letters*, 121(5):056601, 2018
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19. N. N. Intan, **K. Klyukin**, and V. Alexandrov. Theoretical Insights into Oxidation States of Transition Metals at (001) and (111) $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ Spinel Surfaces. *Journal of The Electrochemical Society*, 165(5):A1099–A1103, 2018.
20. S. Ahn, **K. Klyukin**, R. J. Wakeham, J. Rudd, A. R. Lewis, S. Alexander, F. Carla, V. Alexandrov, and E. Andreoli. Poly-amide modified copper foam electrodes for enhanced electrochemical reduction of carbon dioxide. *ACS Catalysis*, 8:4132–4142, 2018.
21. H. Lu, D. Lee, **K. Klyukin**, L.L. Tao, B. Wang, H. Lee, J. Lee, T.R. Paudel, L.-Q. Chen, E.Y. Tsymbal, V. Alexandrov, C.-B. Eom, and A. Gruverman. Tunneling Hot Spots in Ferroelectric SrTiO_3 . *Nano Letters*, 18(1):491–497, 2018.
22. **K. Klyukin** and V. Alexandrov. CO_2 Adsorption and Reactivity on Rutile $\text{TiO}_2(110)$ in Water: An Ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry C*, 121(19):10476–10483, 2017.
23. N.N. Intan, **K. Klyukin**, T.J. Zimudzi, M.A. Hickner, and V. Alexandrov. 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.
24. Z. Jiang, **K. Klyukin**, and V. Alexandrov. First-principles study of adsorption/desorption kinetics of aqueous $\text{V}^{2+}/\text{V}^{3+}$ redox species on graphite in a vanadium redox flow battery. *Physical Chemistry Chemical Physics*, 19(23):14897–14901, 2017.
25. **K. Klyukin** and V. Alexandrov. Effect of intrinsic point defects on ferroelectric polarization behavior of SrTiO_3 . *Physical Review B*, 95(3):035301–035308, 2017.
26. Z. Jiang, **K. Klyukin**, and V. Alexandrov. Structure, hydrolysis, and diffusion of aqueous vanadium ions from Car-Parrinello molecular dynamics. *Journal of Chemical Physics*, 145(11):114303, 2016.
27. **K. Klyukin**, M.G. Shelyapina, and D. Fruchart. DFT calculations of hydrogen diffusion and phase transformations in magnesium. *Journal of Alloys and Compounds*, 644:371–377, 2015.
28. M.G. Shelyapina, A.V. Vyvodtceva, **K. Klyukin**, O.O. Bavrina, Yu.S. Chernyshev, A.F. Privalov, and D. Fruchart. Hydrogen diffusion in metal-hydrogen systems via NMR and DFT. *International Journal of Hydrogen Energy*, 40(47):17038–17050, 2015.
29. **K. Klyukin**, M.G. Shelyapina, and D. Fruchart. Hydrogen induced phase transition in magnesium: an ab initio study. *Journal of Alloys and Compounds*, 580(1):S10–S12, 2013.
30. **K. Klyukin**, M.G. Shelyapina, and D. Fruchart. Modelling of Mg/Ti and Mg/Nb thin films for hydrogen storage. *Solid State Phenomena*, 170:298–301, 2011.

SYNERGISTIC ACTIVITIES

- NSF Panel Reviewer (CMMT/Ceramics)
- Reviewer for Nature Catalysis, Journal of Alloys and Compounds, Applied Physics Letters, International Journal of Hydrogen Energy, Acta Materialia, Physics Letters A, Chemical Physics