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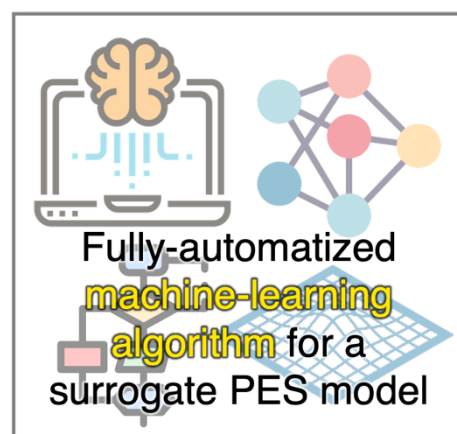
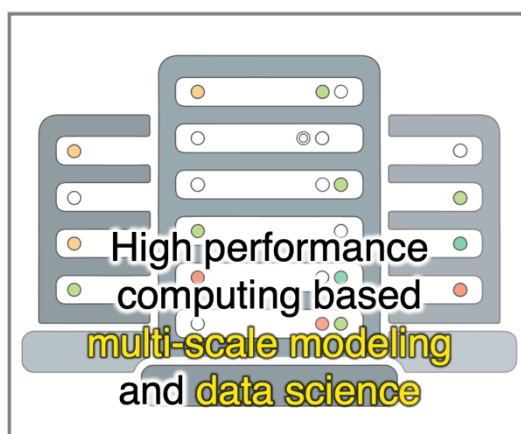
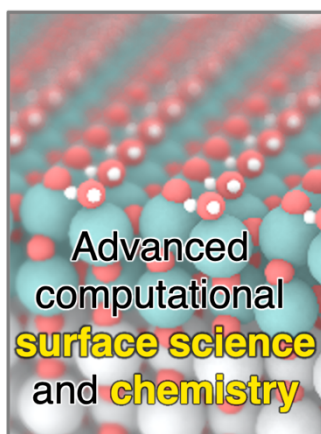
RESEARCH CAREER

Oct 2022 **Postdoctoral Research Fellow**,
 ~ Current *Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft*, Berlin, Germany
 Jan 2021 **Affiliated Research Fellow**,
 ~ Sep 2022 *Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft*, Berlin, Germany

EDUCATION

Dec 2022 **Ph.D. in Chemistry**, *Technische Universität München*, Garching, Germany
Discoveries in Ruthenium Oxide-Based Catalysts
 Supervised by Prof. Karsten Reuter
 Feb 2017 **M.Sc. in Materials Science and Engineering**, *Yonsei University*, Seoul, South Korea
The Opto-Electronic Properties of Hexagonal WO₃: A First-Principles Study,
 Supervised by Prof. Aloysius Soon
 Feb 2015 **B.Sc. in Materials Science and Engineering**, *Yonsei University*, Seoul, South Korea

RESEARCH INTERESTS



PUBLICATIONS

Total **14** peer-reviewed journal publications

1. *B Dopant Evolution in Pd Catalysts After H Evolution/Oxidation Reaction in Alkaline Environment*, Se-Ho Kim, Su-Hyun Yoo, Leonardo Shoji Aota, Ayman El-Zoka, Philwoong Kang, **Yonghyuk Lee**, and Baptiste Gault, *arXiv:2302.02588* (2023)
2. *Black box vs. Grey box: comparing GAP and GPrep-DFTB for Ruthenium and Ruthenium Oxide*, Chiara Panosetti, **Yonghyuk Lee**, Artem Samtsevich, and Christoph Scheurer, *J. Chem. Phys.* 158, 224115 (2023)
3. *Oxidic Structures on Copper-Gold Alloy Nanofacets*, Nandha Kumar, **Yonghyuk Lee**, Giyeok Lee, Sangseob Lee, Taehun Lee, Su-Hyun Yoo, Catherine Stampfl, Aloysius Soon, and Woosun Jang, *Appl. Surf. Sci.* 613, 155913 (2023)
4. *Epitaxial Core-Shell Oxide Nanoparticles: First-principles Evidence for Increased Activity and Stability of Rutile Catalysts for Acidic Oxygen Evolution*, **Yonghyuk Lee**, Christoph Scheurer, and Karsten Reuter, *ChemSusChem* 15, e202200015 (2022)
5. *Data-Efficient Iterative Training of Gaussian Approximation Potentials: Application to Surface Structure*

- Determination of Rutile IrO₂ and RuO₂*, Jakob Timmermann, **Yonghyuk Lee**, Carsten Staacke, Johannes Margraf, Christoph Scheurer, and Karsten Reuter, *J. Chem. Phys.* 155, 244107 (2021)
6. *IrO₂ Surface Complexions Identified through Machine Learning and Surface Investigations*, Jakob Timmermann, Florian Kraushofer, Nikolaus Resch, Peigang Li, Yu Wang, Zhiqiang Mao, Michele Riva, **Yonghyuk Lee**, Carsten Staacke, Michael Schmid, Christoph Scheurer, Gareth S. Parkinson, Ulrike Diebold, and Karsten Reuter, *Phys. Rev. Lett.* 125, 206101 (2020)
 7. *Ruthenium Oxide Nanosheets for Enhanced Oxygen Evolution Catalysis in Acidic Medium*, Sourav Laha, **Yonghyuk Lee**, Filip Podjaski, Daniel Weber, Viola Duppel, Leslie M. Schoop, Florian Pielnhofer, Christoph Scheurer, Kathrin Müller, Ulrich Starke, Karsten Reuter, and Bettina V. Lotsch, *Adv. Energy Mater.* 9, 1803795-1803795 (2019)
 8. *Polytypism in Hexagonal Tungsten Trioxide: Insights from Ab Initio Molecular Dynamics Simulations*, **Yonghyuk Lee**, Taehun Lee, and Aloysius Soon, *J. Phys. Chem. C* 122, 21644-21650 (2018)
 9. *Disentangling the Effects of Inter- and Intra-octahedral Distortions on the Electronic Structure in Binary Metal Trioxides*, Woosun Jang, Jongmin Yun, Taehun Lee, **Yonghyuk Lee**, and Aloysius Soon, *J. Phys. Chem. C* 122, 3558-3566 (2018)
 10. *Aligning the Band Structures of Polymorphic Molybdenum Oxides and Organic Emitters in Light-emitting Diodes*, Jongmin Yun, Woosun Jang, Taehun Lee, **Yonghyuk Lee**, and Aloysius Soon, *Phys. Rev. Applied* 7, 024025 (2017)
 11. *Ab Initio Thermodynamics of Surface Oxide Structures under Controlled Growth Conditions*, Taehun Lee, **Yonghyuk Lee**, Simone Piccinin and Aloysius Soon, *J. Phys. Chem. C* 121, 2228 (2017)
 12. *Understanding the Advantage of Hexagonal WO₃ as an Efficient Photoanode for Solar Water Splitting: A First-principles Perspective*, Taehun Lee†, **Yonghyuk Lee**†, Woosun Jang, and Aloysius Soon, *J. Mater. Chem. A* 4, 11498 (2016) († These authors contributed equally to this work.)
 13. *Unraveling the Intercalation Chemistry of Hexagonal Tungsten Bronze and its Optical Responses*, **Yonghyuk Lee**†, Taehun Lee, Woosun Jang, and Aloysius Soon, *Chem. Mater.* 28, 4528 (2016) († These authors contributed equally to this work)
 14. *In Search of Non-conventional Surface Oxidic Motifs of Cu on Au(111)*, Taehun Lee, **Yonghyuk Lee**, Kisung Kang, and Aloysius Soon, *Phys. Chem. Chem. Phys.* 18, 7349 (2016)

CONTRIBUTED PRESENTATIONS / POSTERS

Total **43** contributions, **16** oral contributions (**3** invited), **27** poster contributions

1. *Application of Gaussian Approximation Potential on Energy Materials Research*, 2023-Spring semester Special Lecture Invitation for Integrated Science and Engineering Division, Underwood International College, Yonsei University, Incheon, Korea (2023), **Yonghyuk Lee (Invited)**
2. *Machine-learning Assisted Surface Structure Determination for Transition Metal Oxide Catalysts*, 15th European Conference on Surface Crystallography and Dynamics (ECSCD15), Grainau, Germany (2023), **Yonghyuk Lee**, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter
3. *Accelerating Theoretical Surface Structure Determination with Machine-Learning Interatomic Potentials: A Case Study on Rutile RuO₂ Surfaces*, The Korean Physical Society (KPS), Daejeon, Korea (2023), **Yonghyuk Lee**, Jakob Timmermann, Carsten Staacke, Johannes Margraf, Christoph Scheurer and Karsten Reuter
4. *Machine-learning Gaussian Approximation Potentials to Discover RuO₂ Surface Reconstructions*, Deutsche Physikalische Gesellschaft e.V. (DPG) Spring meeting, Dresden, Germany (2023), **Yonghyuk Lee**, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter
5. *Layered Iridates for Oxygen Evolution Reaction*, Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis IX, Ringberg, Germany (2023), **Yonghyuk Lee**, Marianne Van der Merwe, Raul Garcia Diez, Christoph Scheurer, and Karsten Reuter
6. *Machine-learning Gaussian Approximation Potentials to Solve a Longstanding Puzzle about RuO₂ Surfaces*, Deutsche Physikalische Gesellschaft e.V. (DPG) Spring meeting, Regensburg, Germany (2022), **Yonghyuk Lee**, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter
7. *Machine-learning Gaussian Approximation Potentials to Solve a Longstanding Puzzle about RuO₂ Surfaces*, Psi-k 2022, Lausanne, Switzerland (2022), **Yonghyuk Lee**, Jakob Timmermann, Chiara

- Panosetti, Christoph Scheurer, and Karsten Reuter
8. *Stable and Cost-efficient Core-shell Catalysts for Enhanced Acidic Oxygen Evolution - A First Principles Approach*, Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis VIII, Dzwirzyno, Poland (2022), **Yonghyuk Lee**, Christoph Scheurer, and Karsten Reuter
 9. *Data-efficient Iterative Training of Machine-Learning Gaussian Approximation Potentials for Surface Structure Determination of Living Heterogeneous Catalysts*, Young Researcher's Workshop on Machine Learning for Materials, Trieste, Italy (2022), **Yonghyuk Lee**, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter
 10. *Stable and Cost-efficient Core-shell Catalysts for Enhanced Acidic Oxygen Evolution - A First Principles Approach*, 31st Topical Meeting of the International Society of Electrochemistry, Aachen, Germany (2022), **Yonghyuk Lee**, Christoph Scheurer, and Karsten Reuter
 11. *Data-Efficient Iterative Training of Gaussian Approximation Potentials: Application to Surface Structure Determination of Rutile IrO_2 and RuO_2* , The Korean Physical Society (KPS), Artificial Intelligence Aided Discovery and Investigation of Novel Nanomaterials, Online, Korea (2022), **Yonghyuk Lee (Invited)**
 12. *Data-efficient Iterative Training of Machine-Learning Gaussian Approximation Potentials for Surface Structure Determination of Living Heterogeneous Catalysts*, From Wind and Solar Energy to Chemical Energy Storage: Understanding and Engineering Catalysis under Dynamic Conditions, Online, Germany (2022), **Yonghyuk Lee**, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter
 13. *Data-Efficient Iterative Training of Machine Learning Interatomic Potentials*, Verein Koreanischer Naturwissenschaftler und Ingenieure in Deutschland (VeKNI) Regular Seminar, Berlin, Germany, **Yonghyuk Lee (Invited)**
 14. *Stable and Cost-efficient Core-shell Catalysts for Enhanced Acidic Oxygen Evolution - A First Principles Approach*, Fall Meeting of Verein Koreanischer Naturwissenschaftler und Ingenieure in Deutschland, Essen, Germany (2021) **Yonghyuk Lee**
 15. *Gaussian Approximation Potentials Unveil the Unknown Global Minima Surface Structures of RuO_2* , Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis VII, Bibow, Germany (2021), **Yonghyuk Lee**, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter
 16. *Stable and Cost-efficient Core-shell Catalysts for Enhanced Acidic Oxygen Evolution—A First Principles Approach*, Deutsche Physikalische Gesellschaft e.V. (DPG) Spring meeting, Online, Germany (2021), **Yonghyuk Lee**, Christoph Scheurer, and Karsten Reuter
 17. *IrO_2 Surface Complexions Identified Through Machine-learned Interatomic Potentials*, Deutsche Physikalische Gesellschaft e.V. (DPG) Spring meeting, Online, Germany (2021), Jakob Timmermann, **Yonghyuk Lee**, Carsten Staacke, Christoph Scheurer, and Karsten Reuter
 18. *Stable and Cost-efficient Core-shell Catalysts for the Electrochemical Oxygen Evolution Reaction*, Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis VI, Bad Gastein, Austria (2020), **Yonghyuk Lee**, Christoph Scheurer, and Karsten Reuter
 19. *Modelling Cost-effective RuO_2 Catalysts for the Electrochemical Oxygen Evolution Reaction via a Core-shell Approach*, Deutsche Physikalische Gesellschaft e.V. (DPG) Spring meeting, Regensburg, Germany (2019), **Yonghyuk Lee**, Daniel Opalka, Christoph Scheurer, and Karsten Reuter
 20. *Systematic Characterization of Metal-supported Ultrathin Copper Oxide Layers from First-principles Calculations*, International Union of Materials Research Societies - International Conference on Electronic Materials 2018 (IUMRS-ICEM 2018), Daejeon, South Korea (2018) Taehun Lee, **Yonghyuk Lee**, Byunghun Lee, Kristián Palotás, and Aloysius Soon
 21. *Ab Initio Thermodynamics of Surface Oxide Structures under Controlled Growth Conditions*, International Union of Materials Research Societies - International Conference on Electronic Materials 2018 (IUMRS-ICEM 2018), Daejeon, South Korea (2018) Taehun Lee, **Yonghyuk Lee**, Simone Piccinin, and Aloysius Soon
 22. *Unraveling the Intercalation Chemistry of Hexagonal Tungsten Bronze and Its Optical Responses*, International Union of Materials Research Societies - International Conference on Electronic Materials 2018 (IUMRS-ICEM 2018), Daejeon, South Korea (2018) **Yonghyuk Lee**, Taehun Lee, Woosun Jang, and Aloysius Soon
 23. *Aligning the Band Structures of Polymorphic Molybdenum Oxides and Organic Emitters in Light-emitting*

- Diodes*, International Union of Materials Research Societies - International Conference on Electronic Materials 2018 (IUMRS-ICEM 2018), Daejeon, South Korea (2018) Jongmin Yun, Woosun Jang, Taehun Lee, **Yonghyuk Lee**, and Aloysius Soon
24. *Ab Initio Thermodynamics of Surface Oxide Structures under Controlled Growth Conditions*, ACCMS-PRO Satellite Meeting, NANO KOREA 2018, Seoul, South Korea (2018) Taehun Lee, **Yonghyuk Lee**, Simone Piccinin, and Aloysius Soon
 25. *Ab Initio Thermodynamics of Surface Oxide Structures under Controlled Growth Conditions*, 16th Workshop on First-Principles Computational Materials Physics, Hsinchu, Taiwan (2018) Taehun Lee, **Yonghyuk Lee**, and Aloysius Soon
 26. *Transition Metal Oxide Catalysts for Cost-effective Hydrogen Fuel Production*, Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis IV, Sperlonga, Italy (2018), **Yonghyuk Lee**, Daniel Opalka, Christoph Scheurer, and Karsten Reuter
 27. *Morphology and Electronic Structure of MnO₂ Nanoparticles from First-principles*, Deutsche Physikalische Gesellschaft e.V. (DPG) Spring meeting, Berlin, Germany (2018), **Yonghyuk Lee**, Jakob Timmermann, Daniel Opalka, and Karsten Reuter
 28. *Ab Initio Thermodynamics of Surface Oxide Structures under Controlled Growth Conditions*, American Physical Society (APS) March Meeting, Los Angeles, USA (2018) Taehun Lee, **Yonghyuk Lee**, Simone Piccinin, and Aloysius Soon
 29. *Systematic Characterization of Metal-supported Ultrathin Copper Oxide Layers from First-principles Calculations*, American Physical Society (APS) March Meeting, Los Angeles, USA (2018) Taehun Lee, **Yonghyuk Lee**, Simone Piccinin, and Aloysius Soon
 30. *Aligning the Band Structures of Polymorphic Molybdenum Oxides and Organic Emitters in Light-emitting Diodes*, Korean Ceramic Society Fall Meeting, Seoul, South Korea (2017) Jongmin Yun, Woosun Jang, Taehun Lee, **Yonghyuk Lee**, and Aloysius Soon
 31. *First-principles Thermodynamics of Thin Oxide Structures on Metal Support under Controlled Growth Conditions*, 15th International Nanotech Symposium & Nano-Convergence Expo (NANO KOREA 2017), Ilsan, South Korea (2017) Taehun Lee, **Yonghyuk Lee**, Simone Piccinin, and Aloysius Soon
 32. *The Role of Polymorphism in Molybdenum Trioxides for Light-emitting Diode Applications*, 15th International Nanotech Symposium & Nano-Convergence Expo (NANO KOREA 2017), Ilsan, South Korea (2017) Jongmin Yun, Woosun Jang, Taehun Lee, **Yonghyuk Lee**, and Aloysius Soon
 33. *A First-principles Understanding of the Structure-property Relationships in Polymorphic MoO₃*, Electronic Materials and Applications (EMA 2017) Conference, Orlando, USA (2017) Jongmin Yun, Woosun Jang, Taehun Lee, **Yonghyuk Lee**, and Aloysius Soon
 34. *Understanding the Advantages of Hexagonal WO₃ as an Efficient Photoanode for Solar Water Splitting: A First-principles Perspective*, Electronic Materials and Applications (EMA 2017) Conference, Orlando, USA (2017) Taehun Lee, **Yonghyuk Lee**, Woosun Jang, and Aloysius Soon
 35. *Tuning the Chemical Potential of Non-equilibrium Surface Systems: The O/Cu/Au Case*, International Conference on Electronic Materials and Nanotechnology for Green Environment 2016 (ENGE 2016), Jeju, South Korea (2016), Taehun Lee, **Yonghyuk Lee**, Simone Piccinin, and Aloysius Soon
 36. *Understanding the Advantage of Hexagonal WO₃ as an Efficient Photoanode for Solar Water Splitting: A First-principles Perspective*, Energy Materials Nanotechnology (EMN) Meeting on Computation and Theory, Las Vegas, USA (2016), **Yonghyuk Lee**, Taehun Lee, Woosun Jang, and Aloysius Soon
 37. *Oxidic Copper on the Au(111) Surface: A Theoretical Surface Science Approach*, American Physical Society (APS) March Meeting, Baltimore, USA (2016), Taehun Lee, **Yonghyuk Lee**, and Aloysius Soon
 38. *A DFT Study of Metastable h-WO₃ surfaces*, American Physical Society (APS) March Meeting, Baltimore, MA, USA (2016), **Yonghyuk Lee**, Taehun Lee, Woosun Jang, and Aloysius Soon
 39. *Microfaceting of Cu₂O and Its Implications in Photochemistry*, American Physical Society (APS) March Meeting, Baltimore, USA (2016), Taehun Lee, **Yonghyuk Lee**, Yunjae Lee, and Aloysius Soon
 40. *Influence of Xc-functionals on the Opto-electronic Properties of WO₃ Polymorphs*, Psi-k 2015 Conference, San Sebastian, Spain (2015), **Yonghyuk Lee**, Taehun Lee, Woosun Jang, and Aloysius Soon
 41. *A First-principles Study of the Mechano-thermodynamics of Super-ultrahard Materials*, The 8th Conference of the Asian Consortium on Computational Materials Science (ACCMS-8), Taipei, Taiwan

(2015), **Yonghyuk Lee**, Ji-Hwan Lee, and Aloysius Soon

42. *A Density-functional Theory Study of the Opto-electronic Properties of Polymorphic WO₃*, The 8th Conference of the Asian Consortium on Computational Materials Science (ACCMS-8), Taipei, Taiwan (2015) Taehun Lee, **Yonghyuk Lee**, Woosun Jang, and Aloysius Soon
43. First-principles Approaches to Phase Stability and Transformation, The Korean Institute of Metals and Materials (KIM) March Meeting, Changwon, Korea (2015), **Yonghyuk Lee**, Ji-Hwan Lee, Aloysius Soon

PATENTS

2021 페로브스카이트 및 준 페로브스카이트 관련 물질의 분석 방법 및 장치, 대한민국 특허 제 10-2299462호

SCHOLARSHIP & AWARDS

2022 Young Scientist Award, The Korean Scientists and Engineers Association (VeKNI e.V.)
 2018 ~ 2022 Scholarship for Doctoral Programme, Deutscher Akademischer Austauschdienst (DAAD)
 2015 ~ 2016 Teaching Assistant Scholarship
 2015 Research Assistant Scholarship
 2014 Yonsei Scholarship of Academic Excellence
 2008 National Science and Technology Scholarship

RESEARCH GRANTS

Principle Investigator

2018 Research Grants-Doctoral Programmes in Germany, Deutscher Akademischer Austauschdienst (DAAD)

Participating Investigator

2022 Next-Generation NET Project, Korean Federation of Science and Technology Societies
 2021 Next-Generation NET Project, Korean Federation of Science and Technology Societies
 2018 ~ Kopernikus Project P2X, Bundesministerium für Bildung und Forschung

REFERENCES

Prof. Karsten Reuter (email: reuter@fhi-berlin.mpg.de)
 Theory department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
 Prof. Aloysius Soon (email: aloysius.soon@yonsei.ac.kr)
 Materials Science and Engineering, Yonsei University, Seoul, Korea
 Prof. Woosun Jang (email: woosunjang@yonsei.ac.kr)
 Integrated Sciences and Engineering, Yonsei University, Incheon, Korea