Taehun Lee

November 29, 2023

Nationality: Korean
Date of Birth: 30/05/1987
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EDUCATION

- Feb 2011: *Bachelor*
  Materials Science and Engineering, Yonsei University, S. Korea
- Aug 2019: *Ph.D.*
  Materials Science and Engineering, Yonsei University, S. Korea
  Supervisor: Prof. Aloysius Soon

CAREER

- Sep 2019 - June 2020: *Postdoctoral Research Associate*
  Materials Science and Engineering, Yonsei University, S. Korea
  Supervisor: Prof. Aloysius Soon
- July 2020 - July 2023: *Postdoctoral Research Associate*
  Chemistry, Princeton University
  Supervisor: Prof. Annabella Selloni
- September 2023 - present: *Assistant Professor*
  Division of Advanced Materials Engineering, Jeonbuk National University, S. Korea

AWARDS & FELLOWSHIP

- 2007 - 2011: *National Science & Technology Scholarship*, KOSAF
- 2012 - 2014: *Global Ph.D. Fellowship*, NRF-KOREA
- 2019 - 2020: *Postdoctoral Researcher Supporting Program*, Yonsei University

MEMBERS

- 2016 - Present: "*Materials Horizons*" Community Board Member

METHODS/ LANGUAGES

- Density-functional theory calculations and *ab initio* molecular dynamics simulations using **VASP**, **quantum espresso**, and **CP2K** packages; **Wannier90** for electronic property calculations
- Construction and usage of atomic interaction potentials based on a deep-neural network from *ab initio* data, using **DeePMD-kit** package (interfaced with **LAMMPS** package for large-scale molecular dynamics)
- Languages: Korean, English, **Python** (with atomic simulation environment (**ASE**) modules), LaTex, (intermediate) Bash script

PUBLICATION LIST

25. **T. Lee** and A. Selloni, *Deep and shallow gap states in reduced and n-type doped m-ZrO_2*, J. Phys. Chem. C 127, 13936 (2023)
24. N. Kumar, Y. Lee, G. Lee, S. Lee, **T. Lee**, S.-H. Yoo, C. Stampfl, A. Soon, W. Jang, *Oxidic structures on copper-gold alloy nanofacets*, Appl. Surf. Sci. 613, 155913 (2023)
23. **T. Lee** and A. Selloni, *Aggregation of oxygen vacancies in anatase and rutile TiO_2*, J. Phys. Chem. C 127, 627 (2023)
22. **T. Lee**,# M. Ferri, S. Piccinin, and A. Selloni,# *Theoretical insights into photoelectrochemical water reduction on delafossite $CuRhO_2$*, ACS Energy Lett. 7, 1528 (2022) (#corresponding author)
21. X. Jin,* K.-G. Lee,* **T. Lee**,* G. Lee, S. M. Oh, A. Soon, and S.-J. Hwang, *Composition-controlled ultrathin holey $TiO_{1-x}N_x$ nanosheets as powerful hybridization matrices for highly mass-efficient electrocatalysts*, Chem. Eng. J. 437, 135415 (2022) (*X. Jin, K.-G. Lee, and T. Lee contributed equally to this work)
20. **T. Lee**,# M. Ferri, S. Piccinin, and A. Selloni,# *Structure, electronic properties and defect chemistry of delafossite $CuRhO_2$ bulk and surfaces*, Chem. Mater. 34, 1567 (2022) (#corresponding author)
19. X. Jin,* **T. Lee**,* W. Tamakloe,* S. B. Patil,* A. Soon, Y.-M. Kang, and S.-J. Hwang, *In-situ defect engineering route to optimize the cationic redox activity of layered double hydroxide nanosheet via strong electronic coupling with holey substrate*, Adv. Sci. 9, 2103368 (2022) (*X. Jin, T. Lee, W. Tamakloe, and S. B. Patil contributed equally to this work)
18. Y.-J. Lee, L. T. Trinh, **T. Lee**, K. Palotás, S.-Y. Jeong, J. Kim, and A. Soon, *Completing the picture of initial oxidation on copper*, Appl. Surf. Sci. 562, 150148 (2021)
17. G. Lee, H. Lee, **T. Lee**,# and A. Soon,# *Defect-mediated ab initio thermodynamics of metastable γ-MoN(001)*, J. Chem. Phys. 154, 064703 (2021) (#corresponding author)
16. G. Lee, Y.-J. Lee, K. Palotás, **T. Lee**,# and A. Soon,# *Atomic structure and work function modulations in two-dimensional ultrathin CuI films on Cu(111) from first principles*, J. Phys. Chem. C 123, 16362 (2020) (#corresponding author)
15. J. Lee, H. Kim, **T. Lee**, W. Jang, K. H. Lee, and A. Soon, *Revisiting polytypism in hexagonal ternary sulfide $ZnIn_2S_4$ for photocatalytic hydrogen production Within the Z-scheme*, Chem. Mater. 31, 4282 (2019)
14. Y.-J. Lee, **T. Lee**, and A. Soon, *Phase stability diagrams of group VI Magnéli oxides and their implications for photon-assisted applications*, Chem. Mater. 31, 4282 (2019)
13. L. T. Trinh,* **T. Lee**,* S. Kim, Y.-J. Lee, G. Duvjir, K. Jang, K. Palotás, S.-Y. Jeong, A. Soon, and J. Kim, *Growing ultrathin Cu_2O films on highly crystalline Cu(111): A closer inspection from microscopy and theory*, J. Phys. Chem. C 123, 12716 (2019) (*L. T. Trinh and T. Lee contributed equally to this work)

12. **T. Lee**, Y.-J. Lee, K. Palotás, G. Lee, C. Stampfl, and A. Soon, *Polymorphic expressions of ultrathin oxidic layers of Mo on Au(111)*, Nanoscale 11, 6023 (2019)
11. Y. Lee,* **T. Lee**,* and A. Soon, *Polytypism in hexagonal tungsten trioxide: Insights from ab initio molecular dynamics simulations*, J. Phys. Chem. C 122, 21644 (2018) (*Y. Lee and T. Lee contributed equally to this work)
10. Y.-J. Lee, **T. Lee**, and A. Soon, Over-stoichiometry in heavy metal oxides: The case of iono-covalent tantalum trioxides, Inorg. Chem. 57, 6057 (2018)
9. W. Jang, J. Yun, **T. Lee**, Y. Lee, and A. Soon, *Disentangling the effects of inter- and intra-octahedral distortions on the electronic structure in binary metal trioxides*, J. Phys. Chem. C 122, 3558 (2018)
8. J.-H. Lee, J. Yun, **T. Lee**, and A. Soon, *Ab initio surface phase diagram of Sn/Cu(001): Reconciling experiments with theory*, Phys. Rev. Applied 8, 034010 (2017)
7. J. Yun, W. Jang, **T. Lee**, Y. Lee, and A. Soon, *Aligning the band structures of polymorphic molybdenum oxides and organic emitters in light-emitting diodes*, Phys. Rev. Applied 7, 024025 (2017)
6. **T. Lee**, Y. Lee, S. Piccinin and A. Soon, *Ab initio thermodynamics of oxidic surface structures under controlled growth conditions*, J. Phys. Chem. C 121, 2228 (2017)
5. **T. Lee**,* Y. Lee,* W. Jang, and A. Soon, *Understanding the advantage of hexagonal WO_3 as an efficient photoanode for solar water splitting: A first-principles perspective*, J. Mater. Chem. A 4, 11498 (2016) (*T. Lee and Y. Lee contributed equally to this work)
4. Y. Lee,* **T. Lee**,* W. Jang, and A. Soon, *Unraveling the intercalation chemistry of hexagonal tungsten bronze and its optical responses*, Chem. Mater. 28, 4528 (2016) (*Y. Lee and T. Lee contributed equally to this work)
3. **T. Lee**, Y. Lee, K. Kang, and A. Soon, *In search of non-conventional surface oxidic motifs of Cu on Au(111)*, Phys. Chem. Chem. Phys. 18, 7349 (2016)
2. R. Q. Zhang, **T. Lee**, B.-D. Yu, C. Stampfl, and A. Soon, *The role of titanium nitride supports for single-atom platinum-based catalysts in fuel cell technology*, Phys. Chem. Chem. Phys. 14, 16552 (2012)
1. **T. Lee**, B. Delley, C. Stampfl, and A. Soon, *Environment-dependent nanomorphology of TiN: Influence of surface vacancies*, Nanoscale 4, 5183 (2012)

REFERENCES

- **Professor Aloysius Soon** (aloysius.soon@yonsei.ac.kr)
  Department of Materials Science and Engineering, Yonsei University, S. Korea
  Relationship: Former supervisor and collaborator
- **Professor Annabella Selloni** (aselloni@princeton.edu)
  Department of Chemistry, Princeton University, US
  Relationship: Former supervisor and collaborator
- **Professor Seong-Ju Hwang** (hwangsju@yonsei.ac.kr)
  Department of Materials Science and Engineering, Yonsei University, S. Korea
  Relationship: Collaborator

CONFERENCES (TALKS)

7. (Invited) Materials Research Society (MRS) Spring Meeting, USA (2022), *Structure and Chemistry of Delafossite $CuRhO_2$*, **T. Lee**, and A. Selloni
6. American Physical Society (APS) March Meeting, USA (2022), *Structure, Electronic Properties and Defect Chemistry of Delafossite $CuRhO_2$ Bulk and Surfaces*, **T. Lee**, M. Ferri, S. Piccinin, and A. Selloni
5. Deutsche Physikalische Gesellschaft e. V. (DPG) Spring Meeting of the Condensed Matter Section (SKM), Germany (2019) *Revisiting the O/Cu(111) system (again): Looking through the lens of theoretical surface spectroscopy and microscopy*, **T. Lee**, Y. Lee, G. Lee, K. Palotás, and A. Soon
4. Korean Physical Society (KPS) Fall Meeting, Korea (2018) *Systematic characterization of metal-supported ultrathin copper oxide layers from first-principles calculations*, **T. Lee**, Y. Lee, K. Palotás, and A. Soon
3. American Physical Society (APS) March Meeting, USA (2018) *Systematic characterization of metal-supported ultrathin copper oxide layers from first-principles calculations*, **T. Lee**, Y. Lee, S. Piccinin, and A. Soon
2. 4th International Conference on Electronic Materials and Nanotechnology for Green Environment (ENGE), Korea (2016), *Tuning the chemical potential of nonequilibrium surface systems: The O/Cu/Au case*, **T. Lee**, Y. Lee, S. Piccinin, and A. Soon
1. American Physical Society (APS) March Meeting, USA (2016), *Oxidic copper on the Au(111) surface: A theoretical surface science approach*, **T. Lee**, Y. Lee, and A. Soon