

### Current Position

2022 – now **Assistant Professor**, Department of Chemical Engineering, National Tsing Hua University, Hsinchu, Taiwan

### Education

- 2016 – 2020 **Ph.D. in Chemistry and Chemical Engineering**, EPFL, Lausanne, Switzerland  
PhD Thesis: Rational Design of Hole Transport Materials: Tools and Structure-Packing-Property Relationships  
Advisor: Prof. Clémence Corminboeuf
- 2013 – 2015 **M.Sc. in Materials Science and Engineering**, National Taiwan University, Taipei, Taiwan  
Master Thesis: Computational Study of the Origins of the Enhanced Li Storage Capacity and the Kinetic Behaviors of Li Ions on Reduced Graphene Oxide  
Advisor: Prof. Chin-Lung Kuo
- 2008 – 2012 **B.Sc. in Materials Science and Engineering**, National Taiwan University, Taipei, Taiwan  
Bachelor Project: Investigation on the Effect of Aluminum Ion on Electrodeposition Behavior of Cr From Cr(III)-Formic Acid Electrolyte  
Advisor: Prof. Chao-Sung Lin

### Academic Employment

- 2022 – now **Assistant Professor**, National Tsing Hua University, Hsinchu, Taiwan
- 2020 – 2022 **Postdoctoral researcher in theory group**, Max Planck Institute for Polymer Research, Mainz, Germany

### Publications

corresponding author\*, applicant, co-first author<sup>†</sup>

23. **Conjugated Microporous Polymers Incorporating Thiazolo [5, 4-d] thiazole Moieties for Sunlight-Driven Hydrogen Production From Water**  
Maha Mohamed Samy, Islam MA Mekhmer, Mohamed Gamal Mohamed\*, Mohamed Hammad Elsayed, [Kun-Han Lin](#), Yi-Kuan Chen, Tien-Lin Wu, Ho-Hsiu Chou\*, Shiao-Wei Kuo\*, *Chem. Eng. Sci.* **446** (2022), 137158.
22. **Virtual Screening for Organic Solar Cells and Light Emitting Diodes**  
Nancy C. Forero-Martinez, [Kun-Han Lin](#), Kurt Kremer and Denis Andrienko\*, *Adv. Sci.* (2022), 2200825.
21. **Virtual screening of TADF emitters for single-layer OLEDs**  
[Kun-Han Lin](#)\*, Gert-Jan A. Wetzelaer, Paul W. Blom, Denis Andrienko\*, *Front. Chem.* **9** (2021), 1080.
20. **Glass transition temperature prediction of disordered molecular solids**  
[Kun-Han Lin](#)\*, Leanne Paterson, Falk May, Denis Andrienko\*, *Npj Comput. Mater.* **7** (2021)
19. **Chemical Design Rules for Non-Fullerene Acceptors in Organic Solar Cells**  
Anastasia Markina, [Kun-Han Lin](#), Wenlan Liu, Carl Poelking, Yuliar Firdaus, Diego Rosas Villalva, Jafar I Khan, Sri HK Paleti, George T Harrison, Julien Gorenflot, Weimin Zhang, Stefaan De Wolf, Iain McCulloch, Thomas D Anthopoulos, Derya Baran, Frédéric Laquai, Denis Andrienko\*, *Adv. Energy Mater.* (2021) 2102363.

18. **Molecular library of OLED host materials—Evaluating the multiscale simulation workflow**  
Anirban Mondal, Leanne Paterson, Jaeyoung Cho, [Kun-Han Lin](#), Bas van der Zee, Gert-Jan A. H. Wetzelaer, Andrei Stankevych, Alexander Vakhnin, Jang-Joo Kim, Andrey Kadashchuk, Paul W. M. Blom, Falk May, and Denis Andrienko\*, *Chem. Phys. Rev.* **2** (2021) 031304.
17. **Catalytic Hydrocracking of Synthetic Polymers into Grid-compatible Gas Streams**  
Wei-Tse Lee, Felix D. Bobbink, Antoine P. van Muyden, [Kun-Han Lin](#), Clémence Corminboeuf, Reza R. Zamani, Paul J. Dyson\*, *Cell Reports Physical Science* **2** (2021) 100332.
16. **Is a Single Conformer Sufficient to Describe the Reorganization Energy of Amorphous Organic Transport Materials?**  
Jacob Terence Blaskovits<sup>†</sup>, [Kun-Han Lin](#)<sup>†</sup>, Raimon Fabregat, Iwona Swiderska, Hélène Wu, Clémence Corminboeuf\*, *J. Phys. Chem. C*, **31** (2021) 17355.
15. **Structure-Property Relationships in Bithiophenes with Hydrogen-Bonded Substituents**  
Bilal Özen, Farzaneh Fadaei Tirani, Kurt Schenk, [Kun-Han Lin](#), Rosario Scopelliti, Clémence Corminboeuf, Holger Frauenrath\*, *Chem. Eur. J.*, **27** (2021) 3348.
14. **FB-ECDA: Fragment-based Electronic Coupling Decomposition Analysis for Organic Amorphous Semiconductors**  
[Kun-Han Lin](#), Clémence Corminboeuf\*, *J. Phys. Chem. A*, **31** (2020) 10624.
13. **Molecular Design and Operational Stability: Toward Stable 3D/2D Perovskite Interlayers**  
Sanghyun Paek, Cristina Roldán-Carmona, Kyung Taek Cho, Marius Franckevičius, Hobeom Kim, Hiroyuke Kanda, Nikita Drigo, [Kun-Han Lin](#), Mingyuan Pei, Rokas Gegevičius, Hyung Joong Yun, Hoichang Yang, Pascal A. Schouwink, Clémence Corminboeuf, Abdullah M. Asiri, Mohammad Khaja Nazeeruddin\*, *Adv. Sci.*, (2020) 2001014.
12. **Direct Observation of Aggregation-Induced Emission Mechanism**  
Jianxin Guan, Rong Wei, Antonio Prlj, Jie Peng, [Kun-Han Lin](#), Jitian Liu, Han Han, Clémence Corminboeuf, Dahui Zhao, Zhihao Yu, Junrong Zheng\*, *Angew. Chem. Int. Ed.*, **59** (2020) 14903.
11. **FB-REDA: Fragment-Based Decomposition Analysis of the Reorganization Energy for Organic Semiconductors**  
[K.-H. Lin](#), C. Corminboeuf\*, *Phys. Chem. Chem. Phys.*, **22** (2020) 11881.
10. **Doped but stable: spirobisacridine hole transporting materials for hysteresis-free and stable perovskite solar cells**  
N. Drigo, C. Roldan-Carmona, M. Franckevičius, [K.-H. Lin](#), R. Gegevičius, H. Kim, P. A. Schouwink, A. A. Sutanto, S. Olthof, M. Sohail, K. Meerholz, V. Gulbinas, C. Corminboeuf, S. Paek, M. K. Nazeeruddin\*, *J. Am. Chem. Soc.*, **142** (2019) 1792.
9. **Getting the Right Twist: Influence of Donor-Acceptor Dihedral Angle on Exciton Kinetics and Singlet-Triplet Gap in Deep Blue Thermally Activated Delayed Fluorescence Emitter**  
S. Weißenseel, N. Drigo, L. Kudriashova, M. Schmid, T. Morgenstern, [K.-H. Lin](#), A. Prlj, C. Corminboeuf, A. Sperlich, W. Brütting, M. K. Nazeeruddin, V. Dyakonov\*, *J. Phys. Chem. C*, **123** (2019) 27778.
8. **Multiarm and Substituent Effects on Charge Transport of Organic Hole Transport Materials**  
[K.-H. Lin](#), A. Prlj, L. Yao, N. Drigo, H.-H. Cho, M. K. Nazeeruddin, K. Sivula, C. Corminboeuf\*, *Chem. Mater.*, **31** (2019) 6605.
7. **Mechanisms of fluorescence quenching in prototypical aggregation-induced emission systems: excited state dynamics with TD-DFTB**  
T. Tran, A. Prlj, [K.-H. Lin](#), D. Hollas, C. Corminboeuf\*, *Phys. Chem. Chem. Phys.*, **21** (2019) 9026.
6. **Read between the Molecules: Computational Insights into Organic Semiconductors**  
G. Gryn'ova, [K.-H. Lin](#), C. Corminboeuf\*, *J. Am. Chem. Soc.*, **140** (2018) 16370.
5. **Restriction Enzyme Analysis of Double-Stranded DNA on Pristine Single-Walled Carbon Nanotubes**  
S.-J. Wu, N. Schuergers, [K.-H. Lin](#), A. J. Gillen, C. Corminboeuf, A. A. Boghossian\*, *ACS Appl. Mater. Interfaces*, **10** (2018) 37386.

4. **How does alkyl chain length modify the properties of triphenylamine-based hole transport materials?**  
K.-H. Lin, A. Prlj, C. Corminboeuf\*, *J. Mater. Chem. C*, **6** (2018) 960.
3. **A Rising Star: Truxene as a Promising Hole Transport Material in Perovskite Solar Cells**  
K.-H. Lin, A. Prlj, C. Corminboeuf\*, *J. Phys. Chem. C*, **121** (2017) 21729.
2. **Lithiation mechanisms and lithium storage capacity of reduced graphene oxide nanoribbons: a first-principles study**  
K.-H. Lin, C.-L. Kuo\*, *J. Mater. Chem. A*, **5** (2017) 4912.
1. **Microstructure and properties of carbon–sulfur-containing chromium deposits electroplated in trivalent chromium baths with thiosalicylic acid**  
C.-W. Chien, C.-L. Liu, F.-J. Chen, K.-H. Lin, C.-S. Lin\*, *Electrochim. Acta*, **72** (2012) 74.

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## Honors & Awards

- 2020 **Early Postdoc.Mobility Fellowship**, *Swiss National Science Foundation*
- 2018 **SCS Travel Award**, *Swiss Chemical Society*
- 2015 **Graduate Student Scholarship**, *Micron Technology Foundation*
- 2011 – 2012 **College Student Research Scholarship**, *National Science Council*, Taiwan
- 2012 **Honorary Member**, *Phi Tau Phi Scholastic Honor Society*
- 2011 **CSC Educational Foundation Scholarship**, *China Steel Cooperation*, Taiwan