



BATJARGAL SAINBILEG

Assistant Research Fellow

Center of Atomic Initiative for New Materials &
Center of Condensed Matter Sciences,
National Taiwan University

CONTACT

📍 Room 731, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan

☎ +886-2-33669478

+886-986831193

✉ batjargal@ntu.edu.tw

sc.batjargal.s@gmail.com

🎓 Google scholar page



SKILLS

- ❖ **DFT, DFPT, AIMD, TDDFT Codes:**
VASP, Quantum ESPRESSO, Phonopy, BoltzTrap, LOBSTER, CRYSTAL17 and Gaussian16
- ❖ **Programming:** Python, Bash shell scripts, Mathematica, R languages
- ❖ **Machine Learning:** Supervised and Unsupervised methods via Google Colab, Jupyter, Kaggle

RESEARCH INTEREST

- ❖ Quantum First-Principles Calculations
- ❖ Theoretical Condensed Matter Physics
- ❖ Nanoscience
- ❖ Semiconductors
- ❖ 2D materials
- ❖ Metal-Organic Frameworks (MOFs)
- ❖ Computational photo(electro) catalysis

RESEARCH EXPERIENCE

Assistant Research Fellow **2023 – present**
Center of Atomic Initiative for New Materials & Center of Condensed Matter Sciences, National Taiwan University (NTU), Taiwan

Postdoctoral Research Fellow **2018 – 2023**
Center of Condensed Matter Sciences, National Taiwan University (NTU), Taiwan

Research Assistant **2011 – 2018**
Center of Condensed Matter Sciences, National Taiwan University (NTU), Taiwan

Researcher **2005 – 2010**
Institute of Physics and Technology, Mongolian Academy of Sciences (MAS), Mongolia

EDUCATION

Ph.D. in Physics **2011 – 2018**
Taiwan International Graduate Program (TIGP), Academia Sinica, Taiwan

M.Sc. in Physics **2005 – 2007**
National University of Mongolia (NUM), Mongolia

B.Sc. in Physics **2001 – 2005**
National University of Mongolia (NUM), Mongolia

PUBLICATION

- (1) May Ngue, C.; Fu Ho, K.; **Sainbileg, B.**; Batsaikhan, E.; Hayashi, M.; Yi Lee, K.; San Chen, R.; Kit Leung, M. Conductivity and photoconductivity in a two-dimensional zinc bis (triarylamine) coordination polymer. *Chem. Sci.* **2023**, 14 (5), 1320–1328.
- (2) Suragtkhuu, S.; Sunderiya, S.; Purevdorj, S.; Bat-Erdene, M.; **Sainbileg, B.**; Hayashi, M.; R. Bati, A. S.; G. Shapter, J.; Davaasambu, S.; Batmunkh, M. Rhenium anchored $Ti_3C_2T_x$ (MXene) Nanosheets for electrocatalytic hydrogen production. *Nanoscale Adv.* **2023**, 5 (2), 349–355.
- (3) Kamal, S.; Inamdar, A. I.; Chiou, K. R.; Pathak, A.; Yibeltal, A. W.; Chen, J.-W.; Liaw, W.-F.; Hayashi, M.; **Sainbileg, B.***; Hung, C.-H.; Lu, K.-L. Semiconducting Paddle-Wheel Metal–Organic Complex with a Compact Cu–S Cage. *J. Phys. Chem. C* **2022**, 126 (14), 6300–6307.
- (4) Inamdar, A. I.; **Sainbileg, B.**; Lin, C.-J.; Usman, M.; Kamal, S.; Chiou, K.-R.; Pathak, A.; Luo, T.-T.; Bayikadi, K. S.; Sankar, R.; Chen, J.-W.; Tseng, T.-W.; Chen, R.-S.; Hayashi, M.; Chiang, M.-H.; Lu, K.-L. Regimented Charge Transport Phenomena in Semiconductive Self-Assembled Rhenium Nanotubes. *ACS Appl. Mater. Interfaces* **2022**, 14 (10), 12423–12433.
- (5) Myagmarsereejid, P.; Bat-Erdene, M.; Bati, A. S. R.; **Sainbileg, B.**; Hayashi, M.; Shapter, J. G.; Zhong, Y. L.; Batmunkh, M. Sulfur-Functionalized Titanium Carbide $Ti_3C_2T_x$ (MXene) Nanosheets Modified Light Absorbers for Ambient Fabrication of Sb_2S_3 Solar Cells. *ACS Appl. Nano Mater.* **2022**, 5 (9), 12107–12116.
- (6) Kamal, S.; Inamdar, A. I.; Chiou, K.-R.; **Sainbileg, B.**; Usman, M.; Chen, J.-W.; Luo, T.-T.; Hayashi, M.; Hung, C.-H.; Liaw, W.-F.; Lu, K.-L. Functional Groups Assisted Tunable Dielectric Permittivity of Guest-Free Zn-Based Coordination Polymers for Gate Dielectrics. *Chemistry – A European Journal*, **2022**, 28, e202103905.
- (7) Bat-Erdene, M.; Batmunkh, M.; **Sainbileg, B.**; Hayashi, M.; Bati, A. S. R.; Qin, J.; Zhao, H.; Zhong, Y. L.; Shapter, J. G. Highly Dispersed Ru Nanoparticles on Boron-Doped $Ti_3C_2T_x$ (MXene) Nanosheets for Synergistic Enhancement of Electrocatalytic Hydrogen Evolution. *Small* **2021**, 17, 2102218.
- (8) Inamdar, A. I.; **Sainbileg, B.**; Kamal, S.; Saheb Bayikadi, K.; Sankar, R.; Tsair Luo, T.; Hayashi, M.; Chiang, M.-H.; Lu, K.-L. Water-Assisted Spin-Flop Antiferromagnetic Behaviour of Hydrophobic Cu-Based Metal–Organic Frameworks. *Dalton Trans.* **2021**, 50, 5754–5758.
- (9) Kamal, S.; Bera, K. P.; Usman, M.; **Sainbileg, B.**; Mendiratta, S.; Pathak, A.; Inamdar, A. I.; Hung, C.-H.; Hayashi, M.; Chen, Y.-F.; Lu, K.-L. Phosphor-Free Electrically Driven White Light Emission from Nanometer-Thick Barium–Organic Framework Films. *ACS Appl. Nano Mater.* **2021**, 4 (3), 2395–2403.
- (10) **Sainbileg, B.**; Batsaikhan, E.; Hayashi, M. Impact of Oxygen Defects on a Ferromagnetic CrI_3 Monolayer. *RSC Adv.* **2020**, 10 (69), 42493–42501.
- (11) Bera, K. P.; Kamal, S.; Inamdar, A. I.; **Sainbileg, B.**; Lin, H.-I.; Liao, Y.-M.; Ghosh, R.; Chang, T.-J.; Lee, Y.-G.; Cheng-Fu, H.; Hsu, Y.-T.; Hayashi, M.; Hung, C.-H.; Luo, T.-T.; Lu, K.-L.; Chen, Y.-F. Intrinsic Ultralow-Threshold Laser Action from Rationally Molecular Design of Metal–Organic Framework Materials. *ACS Appl. Mater. Interfaces* **2020**, 12 (32), 36485–36495.
- (12) Kamal, S.; Ru Chiou, K.; **Sainbileg, B.**; I. Inamdar, A.; Usman, M.; Pathak, A.; Luo, T.-T.; Chen, J.-W.; Hayashi, M.; Hung, C.-H.; Lu, K.-L. Thermally Stable Indium Based Metal–Organic Frameworks with High Dielectric Permittivity. *J. Mater. Chem. C* **2020**, 8 (28), 9724–9733.
- (13) **Sainbileg, B.**; Lai, Y.-R.; Chen, L.-C.; Hayashi, M. The Dual-Defective SnS_2 Monolayers: Promising 2D Photocatalysts for Overall Water Splitting. *Phys. Chem. Chem. Phys.* **2019**, 21 (48), 26292–26300.
- (14) Pathak, A.; Shen, J.-W.; Usman, M.; Wei, L.-F.; Mendiratta, S.; Chang, Y.-S.; **Sainbileg, B.**; Ngue, C.-M.; Chen, R.-S.; Hayashi, M.; Luo, T.-T.; Chen, F.-R.; Chen, K.-H.; Tseng, T.-W.; Chen, L.-C.; Lu, K.-L. Integration of a $(-Cu-S)_n$ Plane in a Metal–Organic Framework Affords High Electrical Conductivity. *Nat. Commun.* **2019**, 10 (1), 1721.
- (15) **Sainbileg, B.**; Hayashi, M. Possible Indirect to Direct Bandgap Transition in SnS_2 via Nickel Doping. *Chem. Phys.* **2019**, 522, 59–64.
- (16) Usman, M.; Bera, K. P.; Haider, G.; **Sainbileg, B.**; Hayashi, M.; Lee, G.-H.; Peng, S.-M.; Chen, Y.-F.; Lu, K.-L. Single-Molecule-Based Electroluminescent Device as Future White Light Source. *ACS Appl. Mater. Interfaces* **2019**, 11 (4), 4084–4092.
- (17) **Sainbileg, B.**; Lan, Y.-B.; Wang, J.-K.; Hayashi, M. Deciphering Anomalous Raman Features of Regioregular Poly(3-Hexylthiophene) in Ordered Aggregation Form. *J. Phys. Chem. C* **2018**, 122 (8), 4224–4231.
- (18) Usman, M.; Mendiratta, S.; **Sainbileg, B.**; Haider, G.; Hayashi, M.; Rao Gade, N.; Chen, J.-W.; Chen, Y.-F.; Lu, K.-L. Semiconductor Behavior of a Three-Dimensional Strontium-Based Metal–Organic Framework. *ACS Appl. Mater. Interfaces* **2015**, 7 (41), 22767–22774.