

# Dominikus Brian

Domi is a ResearchPreneur passionate in advancing scientific literacy in agentic AI systems

**AI Engineering for Science** across digital and physical space. Worked on advanced materials for energy harvesting, theoretical and computational chemistry, quantum dynamics in molecular systems, optogenetics molecules, autonomous laboratory, artificial intelligence, full-stack software development

[\[Vision\]](#)

To be a Gardener of Knowledge

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Research

Experience

## Current Research Focus

Research Intent Model : Agentic Intent Discovery and Prediction for Scientific Research [Project Page](#)

ARTEMIS : Automated Review and Trustworthy Evaluation for Manuscripts in Science [Project Page](#)

Agentic Memory for Continuous, Long-term, and Evolving Scientific Literature Understanding [Project Page](#)

## Publications

**Dominikus Brian**, 2024. "Flying Safer Around Miami: Predictive Machine Learning Model for Real-Time Meteorological Aerodrome Report (METAR), under review. [10.55277/ResearchHub.1z7lu2x3.1](#)

Liu, Zengkui, **Dominikus Brian**, and Xiang Sun, 2024. "PyCTRAMER: a python package for charge transfer rate constant of condensed-phase systems from marcus theory to fermi's golden rule", The Journal of Chemical Physics(6), 161. [10.1063/5.0224524](#)

**Dominikus Brian** and Xiang Sun, 2021. "Charge transfer landscape manifesting structure-rate relationship in the condensed phase via machine learning", The Journal of Physical Chemistry B(125), 48. [10.1021/acs.jpcb.1c08260](#)

**Dominikus Brian** and Xiang Sun, 2021. "Generalized quantum master equation: a tutorial review and recent advances", Chinese Journal of Chemical Physics(5), 34:497-524. [10.1063/1674-0068/cjcp2109157](#)

**Dominikus Brian** and Morteza Eslamian, 2020. "Design and development of a coating device: multiple-droplet drop-casting (MDDC-Alpha)",(3), 91. [10.1063/1.5129699](#)

Hu, Zhubin, **Dominikus Brian**, and Xiang Sun, 2021. "Multi-state harmonic models with globally shared bath for nonadiabatic dynamics in the condensed phase",(12), 155. [10.1063/5.0064763](#)

**Dominikus Brian** and Xiang Sun, 2021. "Linear-response and nonlinear-response formulations of the instantaneous marcus theory for nonequilibrium photoinduced charge transfer", J. Chem. Theory Comput.(4), 17:2065-2079. [10.1021/acs.jctc.0c01250](#)

**Dominikus Brian**, Zengkui Liu, Barry D. Dunietz, Eitan Geva, and Xiang Sun, 2021. "Three-state harmonic models for photoinduced charge transfer",(17), 154. [10.1063/5.0050289](#)

**Dominikus Brian** and Morteza Eslamian, 2019. "Analysis of impact dynamics and deposition of single and multiple pedot:pss solution droplets", Exp Fluids(9), 60. [10.1007/s00348-019-2784-4](#)

**Dominikus Brian**, Mohammad-Reza Ahmadian-Yazdi, Claire M. Bolding, and Morteza Eslamian, 2019. "Impact dynamics and deposition of perovskite droplets on pedot:pss and tio2 coated glass substrates", Experimental Thermal and Fluid Science, 105:181-190. [10.1016/j.exphemflusci.2019.03.021](#)

Gholampour, Nadia, **Dominikus Brian**, and Morteza Eslamian, 2018. "Tailoring characteristics of pedot:pss coated on glass and plastics by ultrasonic substrate vibration post treatment", Coatings(10), 8:337. [10.3390/coatings8100337](#)

## Biography

Dominikus Brian (钟鸿盛) is a researcher, analyst, and engineer passionate in global energy transition and sustainable development. Domi's current main scientific and market research expertise are on future energy system, AI for Science, and organic semiconductors. Domi is an industrious well-rounded researcher trained in both theoretical, computational, and experimental science and engineering covering the field of energy, power, nanotechnology, advanced materials, AI, and machine learning. Domi is an avid reader and gardener living in Shanghai, China.

## Work & Leadership Experience

### LONGi Solar, Central R&D Institute

**03/2023 - Present**

Senior Staff Engineer, Research of Innovation Strategy

In my role as an engineer for research and innovation strategy, I contemplate, survey, and assess various technological roadmap for the future of energy and photovoltaics (PV) material. In particular, I specialized in understanding and developing photovoltaics materials and emerging devices for future energy market. Main research topics are: Integrated PV Thermal System(PVT), Vehicle Integrated Pv(VIPV), Vehicle-to-grid(V2G), Edge Energy system, Smart PV, AI for science : Large-Language Model based scientific literature review and data sourcing, Digitalization and AI-integration into new material research through algorithm and data architecture.

### New York University Shanghai.

**08/2022 - 01/2023**

Member of the Interdisciplinary Colloquium Organizing Committee

The interdisciplinary colloquium (IDC) organizing committee was established to facilitate interdisciplinary interactions among the STEM faculties, postdocs and PhD students, aiming to bring together people with different backgrounds, and brainstorm new research projects. The program developed by the IDC focus on promoting discussion around the future of interdisciplinary research at NYU Shanghai. I am contributing to the committee in my role as a PhD student leadership representative.

### Dept. of Chemistry New York University | Division of Arts and Science NYU Shanghai | NYU-ECNU Center for Computational Chemistry

**09/2020 - 01/2023**

Graduate Research Fellow

Develop computational model and calculation protocol for investigating the conformation and chemical space of organic photovoltaics molecule. Worked with the theoretical background framework for charge transfer and quantum dynamics in condensed phase molecular systems. Performed and develop in-house code, software, and interface for big data analysis, machine learning, and scientific computation. Mastered the basics operation and management of supercomputer platform.

### Coal, Metals, and Mineral Trade Broker Intern

**09/2021 - 12/2022**

ZHF Trade

Work on prospecting, inspection, and dealing of information and lead for coal, metals, and minerals supply from Indonesia. Perform due-diligence on company financial and the coal quality based on certification and analysis proof. Go through and negotiate terms and condition with supplier (Indonesian Miners and Shippers) and end customers (Chinese traders and power plants).



**Vision:** To be a Gardener of Knowledge. **Mission:** Learn more, Do more, Share more. **Personality:** ENFJ-A (16personalities.com). **Top 5 Core character traits:** Coach, Deliverer, Believer, Philomath, Catalyst. (high5test.com) **Language:** English, Chinese, Bahasa Indonesia. Cantonese (learning), German (learning) **Talent Status:** Shanghai City Type A Foreign Talent.

## Education

**09/2020 - 01/2023**

### New York University (NYU)

Chemistry, Theory &amp; Computation (Ph.D Candidate → M.Sc.)

Dissertation topic: Charge Transfer Landscape in the Condensed Phase: Simulation and Modelling of Photoinduced Charge Transfer of Organic Photovoltaics Molecule

**09/2017 - 03/2020**

### University of Michigan - Shanghai Jiao Tong University Joint Institute

Power Engineering and Engineering Thermophysics (M.Sc.)

Master's thesis: Droplet Impact, Spreading, and Wetting of Perovskite and PEDOT: PSS Solutions.

**09/2013 - 07/2017**

### Shandong University of Science and Technology

Chemical Engineering and Technology (B.Sc.)

Bachelor's thesis: Investigation of Self-Cooling Thermoelectric Device for Waste Heat Energy Harvesting.

## Skills

### Computational

C++ ▪ Python ▪ Unix/Linux ▪ HPC ▪ Machine Learning ▪ Git ▪ Jupyter Notebook & Lab ▪ Julia ▪ Machine Learning (scikit-learn, PyTorch, TensorFlow) ▪ Big Data ▪ VMD ▪ AutoCAD ▪ COMSOL ▪ Adobe (Illustrator & Photoshop) ▪ Maya ▪ SOLIDWORKS ▪ ImageJ ▪ FIJI ▪ Origin ▪ MATLAB ▪ Aspen plus ▪ ANSYS ▪ Quantum Chemistry (Gaussian, QChem, Terachem, Turbomole, Orca).

### Experimental

General wet and analytical chemistry ▪ Spray Coating, Spin Coating, and Blade Coating ▪ 3D-printing ▪ Tensiometer ▪ Rheometer ▪ CMOS High-Speed imaging ▪ Surface Profilometry ▪ SEM ▪ XRD ▪ AFM ▪ CLSM ▪ Glovebox ▪ 3D Laser Vibrometer ▪ I-V Curve measurement ▪ UV-vis Spectroscopy .

### Theoretical

Photovoltaics ▪ Fluid Mechanics ▪ Charge Transfer ▪ Thermoelectric ▪ Thin Film Fabrications ▪ Droplet ▪ Wetting and Surface Science ▪ Quantum Mechanics ▪ Soft Matter Physics ▪ Statistical Mechanics ▪ Quantum Chemistry ▪ Material Science ▪ Nanotechnology.

## Interests

- ▶ Future Energy System
- ▶ AI4Science: Digitalization and AI integration for New Material RnD
- ▶ Future PV Materials and Industrialization
- ▶ Digital Twins
- ▶ Energy Surplus Building
- ▶ Autonomous Laboratories
- ▶ Garden & Landscape

### Laboratory of Thin Liquid and Solid Films and Photovoltaics of UM-SJTU

09/2017 - 03/2020

Lab Member, Safety Coordinator, Technical Engineer

Investigation of droplet impact on heated liquid surface. Developing a low-cost and scalable droplet-based thin film fabrication methods and instrument for printing of advanced materials. Droplet impact, spreading, and wetting of Perovskite and PEDOT: PSS and their application in the printing of thin film solar cells.

### Frontier in Innovative Technology (FIT) Young Investigator Symposium at UM-SJTU

09/2019

Participant / Volunteer

Participate in the conference focusing on various advance technology in energy and health. Volunteer in the event organization and reception of invited guest.

### The 3rd International RenDanHeYi Model Forum

09/2019

1-on-1 bilingual interpreter for VIP experts and leaders

Personal assistant to Nobel Laurates Economist, Management thinking leaders attending the conference. Liaison with event organizer.

### The 1st Material Surface & Interface International Academic Forum - Jiangsu University of Technology

04/2019

Invited speaker / Volunteer Facilitator

Invited speaker in the lecture series session. A volunteer facilitator to bridge the communication between invited VIP experts with the organizing committee of the host university.

### SJTU Global Engagement Program – Bangladesh Challenge

11/2018 - 02/2019

Coordinator team member and field trip team leader

Work with the other coordination team members for the planning of the project. Lead team members in the field trip to Thailand and Bangladesh.

### University of Michigan – Shanghai Jiao Tong University Graduate Student Union

07/2018 - 06/2019

Deputy Chairman

Lead the departments of art and sports and coordinate various events in the college.

### Michigan China Center

08/2018 - 09/2018

Market Analyst & Program Assistant

Perform market analysis on the topic of autonomous driving cars. Handle local business development task in China for trade partner from Michigan States.

### Indonesian Students' Association in China (Under the direct jurisdiction of the Indonesian Embassy)

03/2014 - 05/2015

Nationwide Headquarter Deputy Treasurer and Founder & First Chairman of the Qingdao Branch

Established new organization branch in Qingdao city and served more than 12,000 Indonesian students studying in China.

- ▶ Orphan Education
- ▶ Culinary and Pastry
- Swimming, Table Tennis,
- ▶ Tennis, Bowling,
- Volleyball, Ultimate Frisbee

## Test Scores

- ▶ GRE : 314
- ▶ TOEFL : 107
- ▶ IELTS : 7.0
- ▶ HSK 6 : 242
- ▶ HSK 5: 259

## Contact

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## Selected Awards & Honors

New York University (NYU) Shanghai Doctoral Fellowship	2020 - 2024
China Scholarship Council Master degree Full Scholarship Type A for International Student	2017-2020
3rd prize winner - China Global Television Network (CGTN) Belt and Road essay contest	2019
KLA-Tencor Scholarship of UM-SJTU Joint Institute ; U21/PwC Innovation Challenge-Global Finalist	2018

## Publications

- Nadia Gholampour, **Dominikus Brian**, Morteza Eslamian\*, Tailoring Characteristics of PEDOT: PSS Coated on Glass and Plastics by Ultrasonic Substrate Vibration Post Treatment, *Coatings*, 8 (10), 337 (2018).
- Dominikus Brian**, Mohammad-Reza Ahmadian-Yazdi, Claire Barratt, Morteza Eslamian\*, Impact Dynamics and Deposition of Perovskite Droplets on PEDOT: PSS and TiO<sub>2</sub> Coated Glass Substrates, *Exp. Therm. Fluid Sci.*, 105, 181-190 (2019).
- Dominikus Brian**, Morteza Eslamian\*, Analysis of Impact Dynamics and Deposition of Single and Multiple PEDOT: PSS Solution Droplets, *Exp. Fluids*, 60, 1-15 (2019).
- Dominikus Brian**, Morteza Eslamian\*, Design and Development of a Coating Device: Multiple-Droplet Drop-Casting (MDDC-Alpha), *Rev. Sci. Instrum.*, 91, 033902 (2020).
- Dominikus Brian**, Xiang Sun\*, Linear-Response and Nonlinear-Response Formulations of the Instantaneous Marcus Theory for Nonequilibrium Photoinduced Charge Transfer, *J. Chem. Theory Comput.* 17, 2065-2079 (2021).
- Dominikus Brian**, Zengkui Liu, Barry D. Dunietz, Eitan Geva, Xiang Sun\*, Three-State Harmonic Models for Photoinduced Charge Transfer, *J. Chem. Phys.* 154, 174105 (2021).
- Zhubin Hu, **Dominikus Brian**, Xiang Sun\*, Multi-State Harmonic Models with Globally Shared Bath for Nonadiabatic Dynamics in the Condensed Phase, *J. Chem. Phys.* 155, 124105 (2021).
- Dominikus Brian**, Xiang Sun\*, Generalized Quantum Master Equation: A Tutorial Review and Recent Advances, *Chin. J. Chem. Phys.* 34, 5, 497-524 (2021).
- Dominikus Brian**, Xiang Sun\*, Charge Transfer Landscape Manifesting Structure-Rate Relationship in the Condensed Phase via Machine Learning, *J. Phys. Chem. B*, 125, 13267-13278 (2021).

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