Tianyou Li

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Research Interests

I develop structure-aware **probabilistic machine learning** methods to enable sample-efficient **sequential decision-making** (optimization and control) in complex scientific and engineering systems.

Education

Cornell University, M.Eng. in Electrical and Computer Engineering — 08/2024 – 05/2025

- GPA: 4.1/4.3
- Relevant coursework: Random Signals in Communication and Signal Processing, Optimal System Analysis and Design, Robot Learning, Computer Vision, Network Systems & Games

University of Liverpool, B.Eng. in Electrical Engineering — 09/2022 – 07/2024

- GPA 3.94/4.0 (Rank 1/90) | Part of 2 + 2 transnational program

Xi'an Jiaotong-Liverpool University, B.Eng. in Electrical Engineering — 09/2020 – 07/2022

- GPA: 3.94/4.0 (Rank 1/90) | Part of 2 + 2 transnational program
- Award: 2021 University Academic Excellence Award

Publications

Yixin Cao, Li Yin, Tianshi Zhao, **Tianyou Li**, et al., "Perovskite-based optoelectronic systems for neuromorphic computing." *Nano Energy*, 2024, DOI

Research & Project

Gaussian Processes for Uncertainty Quantification of Implicit Functions — 08/2025 – Present

*Research with **Prof. David Bindel**, Cornell University*

- Developed a physics-informed Gaussian Process (GP) to reconstruct latent system energy landscapes from constrained observations of stable states; implemented an augmented covariance matrix to formally condition the GP posterior on observations of energy, zero-gradient, and curvature at equilibrium points.
- Implemented a semi-parametric model by jointly optimizing a quartic mean function with kernel hyperparameters; provided accurate posterior distributions of the system's stable states, enabling an active and safe learning strategy to efficiently map the implicit function by focusing subsequent sampling on critical regions with high uncertainty, such as phase transitions.

Adaptable Microarray Platform for High-Throughput Bayesian Optimization — 05/2025 – Present

*Research with **Dr. Nate Cira**, Cornell University*

- Optimized the TMB-HRP-H_2O_2 enzymatic reaction with adaptable microarray platforms by introducing a slot-constrained encoding for mixed discrete-continuous variables; feasibility is enforced at the encoding layer, eliminating rejection sampling after solving the acquisition function while preserving the surrogate model's capacity to fit mild discontinuities inferred from data.
- Designed neighborhood-augmented Bayesian Optimization (BO) that, for each queried composition, jointly leverages co-printed neighboring wells (near-zero marginal experimental cost) as local perturbations, that accelerate surrogate learning and reduce regret at the same batch size as standard batch BO.

Bayesian Optimization for Reactive Sputtering of Superconducting Thin Films — 05/2025 – Present

*Research with **Dr. Jingjie Yeo**, Cornell University*

- Reproduced a reactive sputtering meta-learning study and fixed its Gaussian Process Regression (GPR) implementation, which neglected inter-feature correlations; replaced it with SAAS-prior GP that automatically selects relevant dimensions, yielding more accurate prediction and better-calibrated uncertainty.
- Benchmarked Attentive Neural Process (ANP) against the paper's meta-learning framework across all reported tasks under identical settings; ANP achieved lower prediction error and more reliable uncertainty (RMSE/R^2 and NLL/MSLL), making it a viable surrogate for subsequent Bayesian optimization.

Transformer-based Any-step Dynamics Model for Model-based RL 01/2025 – 05/2025

Robot Learning Course Project, Cornell University

- Proposed a Transformer-based Any-step Dynamics Model (TADM) that replaces the GRU encoder in ADM with a Transformer encoder; using an anchor state and action subsequences to predict the next state, enabling parallel training / inference and reducing compounding error in long-horizon rollouts without ensembles.
- Observed and hypothesized a tighter error scaling from kL_s to L_s for k-step rollouts; in Hopper-v5, observed faster convergence, lower held-out NLL (0.009), and a return of 2000 within 44k environment steps.

Characterization of LNP Drug Delivery Vehicles by Machine Learning 08/2024 – 05/2025

*M.Eng. Project with **Prof. Peter Doerschuk**, Cornell University*

- Built a physics-informed small-angle X-ray scattering (SAXS) simulator: starting from cryo-EM-based 3D LNP morphologies, used an FFT-based approximation to X-ray scattering intensity under the dilute-solution assumption and injected photon-counting noise via a Poisson model; synthesized mixtures across morphologies and size distributions to produce high-fidelity SAXS for DNN pretraining and evaluation.
- Developed dual-task CNN/ResNet architectures to identify the dominant LNP type and estimate mixture fractions, achieving 96 % accuracy and $R^2 = 0.964$ on held-out SAXS data, providing a scalable screening proxy that reduces reliance on cryo-EM in early-stage quality control.

NFC Device Identification Using Deep Learning and RF Fingerprinting 08/2023 – 06/2024

*B.Eng. Project with **Prof. Junqing Zhang**, University of Liverpool*

- Developed a deep learning pipeline on raw baseband ATQA waveforms, using metric learning strategies to learn robust device-specific embeddings from noisy baseband signals, eliminating handcrafted feature extraction.
- Mitigated position-induced carrier-frequency offset with domain-adversarial training (gradient reversal) on multi-position data; trained a domain-invariant feature extractor while jointly optimizing identity classification and metric-learning losses, preventing representation collapse and achieving robust cross-position generalization with 98.4% identification accuracy (3.38 s per evaluation).

Perovskite-based Optoelectronic Artificial Synaptic TFT 06/2022 – 11/2023

*Research with **Prof. Chun Zhao**, Xi'an Jiaotong-Liverpool University*

- Bridged device physics to learning rules: characterized CsFAMA perovskite synaptic TFTs, (K^+-doped stack with visible-range photoresponse, exhibiting EPSC/IPSC, PPF, STP/LTP), then parameterized ANN/CNN updates by fitting measured LTP/LTD conductance curves into weight-update equations (G^+/G^-) under hardware conductance limits, linking synaptic dynamics to network training.
- Made the device-aware pipeline robust to harmful labels by integrating RDIA-LS, an influence-based relabeling method, into the hardware-constrained networks; on MNIST/CIFAR-10 the RDIA-LS variants remain stable up to 0.8 noise and outperform CE baselines, and a COVID-audio demo shows $\approx 50\%$ accuracy gain at 80% label noise, demonstrating materials-informed ML tolerant to high-noise regimes.

Technical Skills

- **Programming Languages:** Python, MATLAB, C
- **Developer Tools:** Git, GitHub, VS Code, PyCharm
- **Machine Learning**: PyTorch (advanced), TensorFlow, Keras, scikit-learn, HuggingFace
- **Bayesian Optimization**: BoTorch, Gryffin, BoFire
- **Reinforcement Learning**: OpenAI Gym, D4RL, NeoRL, Stable-Baselines3