Liqun "Zoe" Peng, Ph.D.

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Summary

Computational energy systems researcher with a Princeton Ph.D. and 3+ years post-PhD experience developing models and decision-support tools for power systems, low-carbon technologies, and infrastructure planning. Combines mathematical optimization, techno-economic and geospatial analysis, and policy modeling, with recent work extending these capabilities to multi-agent AI systems for grid planning and large loads.

Professional Experience

Assistant Research Scientist **UC Berkeley** **Jan 2026 – Present**

- Serve as Principal Investigator and technical lead on U.S. Department of Energy funded research with LBNL, leading modeling and decision-support work for grid planning, large loads, and emerging energy infrastructure.
- Lead computational research spanning applied AI, large-scale optimization, and energy-infrastructure planning, with ownership of problem formulation, model design, validation, and technical delivery.

Postdoctoral Researcher **Lawrence Berkeley National Lab** **Jan 2023 – Jan 2026**

- Led modeling and analysis across four externally funded energy-system programs, from problem formulation and model development through technical delivery and presentations to funders and research partners.
- Translated policy and infrastructure questions into quantitative modeling workflows and presented results directly to funders, research partners, and technical collaborators.

Applied AI and Energy Optimization

Multi-Agent AI Platform for Grid Planning and Large Loads **2026 – Present**

- Architected a multi-agent AI copilot for grid planning and large-load analysis, orchestrating interconnection, infrastructure, regulatory, and power-system specialists through stateful routing and hybrid retrieval.
- Integrated specialist agents with structured domain datasets and engineering tools through schema-based tool calling, persistent session and project state, and grounded retrieval over a continuously expanding technical and regulatory knowledge base.
- Designed an evaluation and regression-testing harness for cross-model benchmarking, using fixed test sets and blind scoring to evaluate retrieval, routing, tool-use correctness, and response quality.

Offshore Wind-Powered AI Data Center Siting **2025 – Present**

- Formulated a global infrastructure-siting model for offshore wind-powered AI data centers, coupling project-level wind resources, hourly reliability, storage, and network latency to evaluate deployment of GW-scale clean compute.
- Scaled a 43M-variable hourly capacity-expansion and dispatch LP in Linopy and Gurobi through exact regional decomposition, co-optimizing offshore wind, batteries, hydrogen storage, and grid backup at high modeled reliability.
- Designed a latency-qualified compute metric and counterfactual layer linking siting decisions to demand reach, grid-interconnection needs, infrastructure materials, water use, and time-to-power.

Large-Scale Spatial Optimization for Industrial Decarbonization **2024 – 2026**

- Built a national-scale spatiotemporal optimization framework across 548 steel, ammonia, and methanol plants, integrating plant-level industrial data with 25 by 25 km, hourly renewable resources to optimize energy sourcing, electrolysis, storage and grid use.
- Integrated geospatial plant data, hourly time series, and optimization outputs into a decision pipeline for joint multi-sector resource allocation, counterfactual analysis, and robustness testing.
- Implemented plant-level pathway screening across H_2, CCS, and EAF alternatives, translating model outputs into least-cost technology choices and regional deployment priorities.

Applied AI and Energy Optimization

Power System Planning and Regional Decarbonization **2023 – 2026**

- Built hourly, multi-decade power-system planning models to evaluate transmission, regional coordination, shared reserves, storage, and alternative deep-decarbonization pathways.
- Quantified how spatial heterogeneity in resources, load, and generation mix reshapes the value of low-carbon technologies, informing region-specific infrastructure and policy strategies for offshore wind, transport electrification, and grid decarbonization.

Education

- **Princeton University** – Ph.D., *Science, Technology, and Environmental Policy* **2017–2023**
- **Tsinghua University** – M.S., *Environmental Science and Engineering* **2013–2016**
- **Beijing Forestry University** – B.S., *Liang Xi honors research track* **2009–2013**

Technical Skills

- **AI Systems**: Multi-agent orchestration (LangGraph), stateful workflows and memory, schema-based tool calling, hybrid RAG (ChromaDB, BM25, RRF), agent evaluation and regression testing
- **Optimization and Decision Modeling**: LP/MILP, large-scale spatiotemporal optimization, capacity expansion and dispatch, decomposition, resource allocation, spatial optimization, scenario and counterfactual analysis; Gurobi, Linopy
- **Power and Energy Systems**: Grid planning, production-cost modeling, renewable and storage integration, resource adequacy, transmission and interconnection, large-load planning; GridPath, SWITCH-China, PLEXOS
- **Programming**: Python, pandas, NumPy, scikit-learn, Shell

Research Impact and Technical Communication

- Published 20 peer-reviewed papers with 4,200 citations, including first-author work in *Nature Communications*, *One Earth*, and *Communications Earth & Environment*.
- Invited speaker at the University of Cambridge, Baruch College (CUNY), Global Energy Monitor, and other research institutions; Presented energy modeling research at MES, AGU, C3E, and Princeton Andlinger Center meetings, receiving a Best Poster Award.
- Organized an open-modeling workshop spanning nine institutions in China and the United States; served as guest editor for *npj Clean Energy* and reviewer for Nature Portfolio journals and other leading energy and sustainability journals.

Selected First-Author Publications

- **L. Peng**, D. L. Mauzerall, Y. D. Zhong, et al. "Heterogeneous effects of battery storage deployment strategies on decarbonization of provincial power systems in China." *Nature Communications* 2023. Link
- **L. Peng**, G. He, N. Abhyankar, et al. "Aligning offshore wind deployment with local priorities to accelerate power system decarbonization." *Communications Earth & Environment* 2026. Link
- **L. Peng**, Y. Guo, S. Liu, et al. "Subsidizing grid-based electrolytic hydrogen will increase greenhouse gas emissions in coal dominated power systems." *Environmental Science & Technology* 2024. **Best Paper Award, first joint runner-up**. Link
- **L. Peng**, F. Liu, M. Zhou, et al. "Alternative-energy-vehicles deployment delivers climate, air quality, and health co-benefits when coupled with decarbonizing power generation in China." *One Earth* 2021. Link
- **L. Peng**, J. Liu, D. Zhang, et al. "Strategies for decarbonizing steel, ammonia, and methanol plants using low-carbon hydrogen." *Nature Energy*, second-round review.