Thomas J. L. Mustard, Ph.D.

Staff Technical Product Manager

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Summary

Product leader at the intersection of deep computational science, AI platform strategy, and drug discovery. Proven track record of translating proprietary scientific capabilities, from Large Quantitative Models to DFT-based screening workflows, into standardized, enterprise-ready products. Builds and ships at the interface of ML engineering, computational chemistry, and life sciences, closing the loop from experiment to model to actionable decision. A skilled cross-functional leader who speaks the language of the scientist, the ML engineer, and the C-suite without bluffing in any of those rooms.

Experience

Staff Technical Product Manager

SandboxAQ Jan 2025 -- Present

- Defined the product vision and multi-quarter roadmap for a foundational Agentic AI platform designed to be agnostic, serving both the company's drug and materials discovery divisions and aligning engineering efforts with C-level business objectives.
- Architects parallel R&D operating models that synchronize scientific exploration with commercial product readiness to accelerate time-to-market. Established a hybrid release strategy balancing public scientific thought leadership with IP-protected revenue streams.
- Deploys proprietary multi-agent systems as the primary consumption layer for AI Building Blocks, facilitating dynamic composition of models and data APIs to enable customers to solve complex, multi-step scientific problems.
- Defines the roadmap for Model Context Protocol (MCP) servers, positioning proprietary models as specialized, domain-specific tools that foundational LLMs (e.g., Anthropic, Gemini, OpenAI) call dynamically.
- Prototyped and defined the UX for a multi-agent drug discovery workflow system, designing a chat interface that enables medicinal chemists and molecular design scientists to execute complex multi-step computational workflows through natural language prompts. Defined interaction patterns within existing design system guidelines to make advanced AI inference capabilities accessible to non-computational experts.
- Defining the output specification for a proprietary MCP computational tool that returns multiple conformational poses per calculation, surfacing not only the lowest-energy structure but the full ensemble with relative energies, per-atom statistical information, and Boltzmann-weighted averages to quantify prediction uncertainty. This output design enables scientists to interpret model confidence directly within their workflow without requiring computational expertise.
- Architected and deployed an AI-powered invention disclosure workflow that transformed document generation from a 2-week manual process to a sub-1-day automated pipeline, standardizing structure, improving accuracy, and enabling the IP team to scale throughput without adding headcount.

Technical Product Manager (Principal Scientist II)

Schrödinger Jun 2015 -- Jan 2025

- Defined and executed the product vision, strategy, and roadmap for the catalysis and reactivity portfolio. Spearheaded the creation and launch of the flagship AutoRW automated workflow from initial concept through market launch, securing customer co-funding by pitching the full end-to-end vision. Prior to AutoRW, fewer than 100 people worldwide were properly trained to perform computational catalyst screening manually; AutoRW democratized the workflow, enabling bench chemists to test 10x more candidates at 10-20% of their working hours. The AutoRW lineage culminated in the RxnEnumProfiler, a next-generation catalyst design framework published on ChemRxiv (2025), on which Thomas holds last-author credit formally recognizing him as the originator and conceptualizer of the entire workflow.
- Demonstrated AutoRW's enterprise scalability through rigorous benchmarking, showing enterprise deployment enabled screening of 2,000+ catalysts per year at approximately 12x cost efficiency versus experimental synthesis and testing. These metrics directly informed GTM positioning and customer ROI conversations.
- Trained and supported pharma and biotech clients across the full DMTA cycle within LiveDesign, covering structure generation via R-group and reaction-based enumeration, property calculation workflows including docking, QSPR ML models, and FEP, and downstream analysis tooling enabling multiple in silico design-test-analyze iterations before committing to wet-lab synthesis. Directly engaged with medicinal chemists and molecular design scientists to translate computational capabilities into accelerated small molecule programs.

- Executed a structured four-stage product discovery process for new features, covering informal discovery sessions to establish baseline user needs, formal stakeholder interviews capturing requirements and must-have priorities, storyboard-driven presentations to engineering communicating user stories visually alongside product briefs, and coordinated alignment meetings with engineering leads and subject matter experts producing official PRD documents driving ticket generation and engineering sprints.
- Partnered directly with synthetic chemists and computational scientists to co-design the AutoRW user interface within LiveDesign, iteratively refining workflow structure, button placement, and nomenclature through hands-on customer sessions to ensure the UI was intuitive for bench chemists with no prior computational expertise.
- Led the successful integration of AutoRW into the LiveDesign enterprise SaaS platform, securing deployments with Fortune 50 clients and establishing the company's position in the catalysis market.
- Built the catalysis market vertical from the ground up, establishing Schrödinger's presence in homogeneous and organometallic catalysis through hands-on customer engagements, scientific demonstrations, and product co-development. This foundational work directly led to a promotion into product management for the catalysis and reactivity portfolio.

Graduate Research Assistant

Oregon State University — Sep 2010 -- Jun 2015

- Designed and built Eta_Scripts, an open-source automation framework including nPersistentOTS.py (automated transition state searching via rules-based energy tracking) and nMap.py (semi-automated reaction coordinate mapping via 3D fragment swapping), which streamlined DFT input file generation across multiple quantum chemistry engines and seeded the automated catalysis screening concepts that directly prefigured AutoRW.
- Applied DFT to elucidate mechanisms and origins of selectivity in transition-metal-catalyzed reactions (Rh, Cu, Pd), establishing computational models for catalyst efficiency and stereocontrol validated through experimental collaborations and published in JACS, ACS Catalysis, and Angewandte Chemie.
- Conducted free energy perturbation (FEP) and molecular dynamics (MD) simulations on rifampicin derivatives to evaluate binding affinities, building early multiscale simulation experience that later informed hybrid MD/DFT workflows.

Skills

agentic ai	Agentic Workflows, Model Context Protocol (MCP), Large Quantitative Models (LQMs), A2A (Agent-to-Agent) Interactions, API-First Microservices
product strategy	Product Strategy, Product Vision, Product Road Mapping, Go-to-Market (GTM) Strategy
leadership	Cross-functional Team Leadership, Stakeholder Management, Technical Project Management
computational methods	Density Functional Theory (DFT), Molecular Dynamics (MD), Free Energy Perturbation (FEP), Multiscale Simulation (MD/DFT)
technical scientific	AI / Generative AI, Computational Chemistry, Materials & Drug Discovery, Applied Machine Learning, Cheminformatics, QSAR/QSPR Modeling, Molecular Modeling

Education

Oregon State University

Ph.D. in Chemistry

- Specialized in automating and enhanced efficiency of organometallic catalysis mechanism elucidation and materials property prediction

Eastern Washington University

B.S. in Chemistry

Patents / Inventions

"Generating Traces Representing Operations of Multi-Agent Artificial Intelligence Systems". Patent Pending (Filed Dec 2, 2025).

"Generating and Executing Computational Graphs Using Artificial Intelligence Agents". Patent Pending (Filed Dec 4, 2025).

"Optimizing Execution of Computational Graphs". Filing Imminent.

Selected Publications

Dub, P. A.; Hughes, T.; Mustard, T. "A Software Framework for Physics- and AI-Driven Homogeneous Catalyst Design and Reactivity Optimization" ChemRxiv, 2025. DOI:10.26434/chemrxiv-2025-mm69d

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Wills, L. A.; Qu, X.; Chang, I. Y.; Mustard, T. J.; Keszler, D. A.; Persson, K. A.; Cheong, P. H. Y. "Group additivity-Pourbaix diagrams advocate thermodynamically stable nanoscale clusters in aqueous environments" Nature communications, 2017, 8, 1-7. DOI:10.1038/ncomms15852

Tsuchiya, Y.; Tsuji, K.; Inada, K.; Bencheikh, F.; Geng, Y.; Kwak, H. S.; Mustard, T. J.; Halls, M. D.; Nakanotani, H.; Adachi, C. "Molecular design based on donor-weak donor scaffold for blue thermally-activated delayed fluorescence designed by combinatorial DFT calculations." Frontiers in Chemistry, 2020, 8, 403. DOI:10.3389/fchem.2020.00403

Matsuzawa, N. N.; Arai, H.; Sasago, M.; Fujii, E.; Goldberg, A.; Mustard, T. J.; Kwak, H. S.; Giesen, D. J.; Ranalli, F.; Halls, M. D. "Massive theoretical screen of hole conducting organic materials in the heteroacene family by using a cloud-computing environment" The Journal of Physical Chemistry A, 2020, 124, 1981-1992. DOI:10.1021/acs.jpca.9b10998

Mustard, T. J. L.; Afzal, M. A. F.; Sanders, J. M.; Kwak, S. H.; Christensen, S.; Browning, A.; Halls, M. D. "Multiscale modeling of polymers: Leveraging reaction kinetics for structural morphology and property prediction" Sampe neXus, 2021. DOI:TP21-0000000545

Sanders, J. M.; Misra, M.; Mustard, T. J.; Giesen, D. J.; Zhang, T.; Shelley, J.; Halls, M. D. "Characterizing moisture uptake and plasticization effects of water on amorphous amylose starch models using molecular dynamics methods" Carbohydrate Polymers, 2021, 252, 117161. DOI:10.1016/j.carbpol.2020.117161

Mattson, E. C.; Cabrera, Y.; Rupich, S. M.; Wang, Y.; Oyekan, K. A.; Mustard, T. J.; Halls, M. D.; Bechtel, H. A.; Martin, M. C.; Chabal, Y. J. "Chemical modification mechanisms in hybrid hafnium oxo-methacrylate nanocluster photoresists for extreme ultraviolet patterning" Chemistry of Materials, 2018, 30, 6192-6206. DOI:10.1021/acs.chemmater.8b03149