CURRICULUM VITAE

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PERFIL PROFESIONAL

Nacionalidad: Mexicana

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PUBLICACIONES CIENTÍFICAS (43)

1. Mapping uncertainty using differentiable programming
Aiche Journal (2025)

2. Towards agentic science for advancing scientific discovery
Nature Machine Intelligence (2025)

3. Spin-informed universal graph neural networks for simulating magnetic ordering
Proceedings of the National Academy of Sciences of the United States of America (2025)

4. Solving an inverse problem with generative models
Digital Discovery (2025)

5. A classification-based methodology for the estimation of binary surfactant critical micelle concentrations
Digital Discovery (2025)

6. Integrated Systems-to-Atoms (S2A) Framework for Designing Resilient and Efficient Hydrogen Infrastructure Solutions
Energy and Fuels (2025)

7. CatTSunami: Accelerating Transition State Energy Calculations with Pretrained Graph Neural Networks
ACS Catalysis (2025)

8. Multiscale optimization of formic acid dehydrogenation process via linear model decision tree surrogates
Computers and Chemical Engineering (2025)

9. Accessing Numerical Energy Hessians with Graph Neural Network Potentials and Their Application in Heterogeneous Catalysis
Journal of Physical Chemistry C (2025)

10. Autonomous catalysis research with human–AI–robot collaboration
Nature Catalysis (2025)