

# Juan Manuel Islas Islas

Email: docente@utte.edu.mx

ORCID: 0000-0001-6681-7919

## DATOS GENERALES

**CURP:** qweqwewq

**RFC:** wswqeqwe

**Nacionalidad:** Mexicana

**Fecha de Nacimiento:** 28/11/2025

## ARTÍCULOS CIENTÍFICOS

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2. Xin H.. (2025). **Towards agentic science for advancing scientific discovery.** *Nature Machine Intelligence*. DOI: 10.1038/s42256-025-01110-x
3. Xu W.. (2025). **Spin-informed universal graph neural networks for simulating magnetic ordering.** *Proceedings of the National Academy of Sciences of the United States of America*. DOI: 10.1073/pnas.2422973122
4. Kitchin J.R.. (2025). **Solving an inverse problem with generative models.** *Digital Discovery*. DOI: 10.1039/d5dd00137d
5. Chilkunda C.R.. (2025). **A classification-based methodology for the estimation of binary surfactant critical micelle concentrations.** *Digital Discovery*. DOI: 10.1039/d5dd00058k
6. Yuan M.. (2025). **Integrated Systems-to-Atoms (S2A) Framework for Designing Resilient and Efficient Hydrogen Infrastructure Solutions.** *Energy and Fuels*. DOI: 10.1021/acs.energyfuels.4c05903
7. Wander B.. (2025). **CatTSunami: Accelerating Transition State Energy Calculations with Pretrained Graph Neural Networks.** *ACS Catalysis*. DOI: 10.1021/acscatal.4c04272
8. Sunshine E.M.. (2025). **Multiscale optimization of formic acid dehydrogenation process via linear model decision tree surrogates.** *Computers and Chemical Engineering*. DOI: 10.1016/j.compchemeng.2024.108921
9. Wander B.. (2025). **Accessing Numerical Energy Hessians with Graph Neural Network Potentials and Their Application in Heterogeneous Catalysis.** *Journal of Physical Chemistry C*. DOI: 10.1021/acs.jpcc.4c07477
10. Orouji N.. (2025). **Autonomous catalysis research with human–AI–robot collaboration.** *Nature Catalysis*. DOI: 10.1038/s41929-025-01430-6
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14. Huang Y.. (2024). **Unifying theory of electronic descriptors of metal surfaces upon perturbation.** *Physical Review B*. DOI: 10.1103/PhysRevB.110.L121404
15. Bender J.T.. (2024). **The Potential of Zero Total Charge Predicts Cation Effects for the Oxygen Reduction Reaction.** *ACS Energy Letters*. DOI: 10.1021/acsenergylett.4c01897
16. Abdelmaqsoud K.. (2024). **Structure Sensitive Reaction Kinetics of Chiral Molecules on Intrinsically Chiral Surfaces.** *Journal of Physical Chemistry C*. DOI: 10.1021/acs.jpcc.4c04224
17. Abdelmaqsoud K.. (2024). **Investigating the error imbalance of large-scale machine learning potentials in catalysis.** *Catalysis Science and Technology*. DOI: 10.1039/d4cy00615a
18. Broderick K.. (2024). **Surface Segregation Studies in Ternary Noble Metal Alloys: Comparing DFT and Machine Learning with Experimental Data.** *Chemphyschem*. DOI: 10.1002/cphc.202400073
19. Abed J.. (2024). **Pourbaix Machine Learning Framework Identifies Acidic Water Oxidation Catalysts Exhibiting Suppressed Ruthenium Dissolution.** *Journal of the American Chemical Society*. DOI: 10.1021/jacs.4c01353
20. Tedesco C.C.. (2024). **Cyclic Steady-State Simulation and Waveform Design for Dynamic/Programmable Catalysis.** *Journal of Physical Chemistry C*. DOI: 10.1021/acs.jpcc.4c01543
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