Alejandro Peña-Torres

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Education

2008-2012 B.Sc. Chemistry, National University of Colombia, Bogotá, Colombia.
Research project: Electronic structure study of atoms and molecules in fullerenes using model potentials.

2013-2015 M.Sc. Chemistry, National University of Colombia, Bogotá, Colombia.
Dissertation title: Theoretical development of Coupled Cluster methods under the Any Particle Molecular Orbital frame and its implementation in LOWDIN.

2016-2018 Joint PhD program
PhD in Chemical Physics, University of Bordeaux, Bordeaux, France.
PhD in Physics of Nanostructures and Advanced Materials, University of the Basque Country, Donostia-San Sebastián, Spain.
Thesis title: Contribution to the theoretical description of N_2 dynamics on W(100).

Employment

2019- Postdoctoral Researcher, University of Iceland, Reykjavík, Iceland
Research experience: Atomistic simulations including periodic DFT calculations, molecular dynamics, adaptive kinetic Monte Carlo (AKMC), and the development and application of machine learning potentials to study atomic-scale processes across diverse systems.

2025- System Manager, Division of Information Technology, University of Iceland, Reykjavík, Iceland.
Member of the Icelandic Research e-Infrastructure (IREI) team.
Tasks: User support services for the Icelandic High Performance Computing Centre (IHPC) and research outreach initiatives.

Grants

2014 Grant "Jóvenes Investigadores". Colciencias grant number 617 awarded to young researchers under the project "Explicitely correlated propagator methods for the study of positronic molecules using the any particle molecular orbital theory", Bogotá, Colombia.

2016 Grant "IdEx". Awarded within the International Doctoral Program of the Excellence Initiative (IdEx) of the university of Bordeaux for the project "Theoretical contribution to the description of heterogeneous elementary processes: Hot-Atom dynamics" in the framework of a collaboration with the University of Basque country (Spain), Bordeaux, France

Teaching

2014 TA. Principles of Organic Chemistry laboratory (National University of Colombia, Bogotá, Colombia)

2015 Theoretical and Computational Chemistry (University of Applied and Environmental Sciences, Bogotá, Colombia)

2024 Thermodynamics and Introduction to Statistical Mechanics (University of Iceland, Reykjavík, Iceland)

2025 Molecular Spectroscopy and Reaction Dynamics (University of Iceland, Reykjavík, Iceland)

Selected Publications

1. Peña-Torres, A., Ali, A., Stamatakis, M., Jónsson, H. *Indirect Mechanism of Au adatom diffusion on the Si(100) surface*, Phys. Rev. B. 105, 205411, (2022)

2. Christiansen, M. A. H., Peña-Torres, A., Jónsson, E. Ö., Jónsson, H. *Single-atom substituents in copper surfaces may adsorb multiple CO molecules*, J. Chem. Phys. Lett. 15(21), 5654–5658, (2024)

3. Goswami, A., Peña-Torres, A., Jónsson, E. Ö., Egorov, S. A., Jónsson, H. *Evidence of sharp transitions between octahedral and capped trigonal prism states of the solvation shell of the aqueous Fe^{3+} ion*, J. Phys. Chem. Lett. 15(17), 4523–4530, (2024)

4. Goswami, R., Masterov, M., Kamath, S., Peña-Torres, A., Jónsson, H. *Efficient Implementation of Gaussian Process Regression Accelerated Saddle Point Searches with Application to Molecular Reactions*, arXiv preprint, arXiv:2505.12519 (2025)

5. Peña-Torres, A., Stamatakis, M., Jónsson, H. *Dimerization of Ag adatoms on Si(100) at surprisingly low temperature due to adatom migration on top of Si-dimer rows*, arXiv preprint, arXiv:2506.08207 (2025)