Iñigo Iribarren Aguirre

Postdoctoral researcher in computational chemistry

inigo.iribarren@tum.de iribirii.github.io Munich, Germany iribirii

iñigo-iribarren-aguirre-22884228 Google Scholar 0000-0003-0373-8687 iiribarren.bsky.social

Summary

Computational chemist developing machine learning–powered approaches to design and understand supramolecular metallacages as drug-delivery systems. Background in organocatalysis, noncovalent interactions, and scientific visualization.

Education

Postdoctoral researcher — **Technical University of Munich**, School of Natural Sciences — Munich, Germany — Jan 2024 – present

Ph.D. — **Trinity College Dublin**, School of Chemistry — Dublin, Ireland — Jan 2019 – Jan 2024

M.Sc. — **Universidad Autónoma de Madrid**, Theoretical Chemistry and Computational Modelling (TCCM) — Madrid, Spain — Jan 2016 – Jan 2018

B.Sc. — **Universidad Autónoma de Madrid**, Department of Chemistry — Madrid, Spain — Jan 2012 – Jan 2016

Outreach

SciLab Deutsches Museum (TUM 150th anniversary) — **Public engagement**, Public engagement — Munich, Germany — Jan 2026

Open Day Garching — **Public engagement**, Public engagement — Garching, Germany — Jan 2026

Current Chemistry Investigators — **Primary and secondary school outreach**, Primary and secondary school outreach — Dublin, Ireland — Jan 2021 – Jan 2024

ESB Science Blast	**Public engagement**, Public engagement	Dublin, Ireland Jan 2023
Stories from the lab	**Primary and secondary school outreach**, Primary and secondary school outreach	Dublin, Ireland Jan 2020 – Jan 2021
European Researchers' Night	**Public engagement**, Public engagement	Dublin, Ireland Jan 2020
Spectroscopy in a Suitcase	**Primary and secondary school outreach**, Primary and secondary school outreach	Dublin, Ireland Jan 2019 – Jan 2020

Awards

Best Contributed Talk Jan 2026
European Symposium on Chemical Bonding (CBOND2026) — A Dynamic Evaluation of Cisplatin Encapsulation into $[Pd_2L_4]^{4+}$ Metallacages in Solution

BOC Gases bursary thesis competition — 2nd prize Jan 2024
Trinity College Dublin / BOC Gases

Best poster Jan 2022
3rd European Symposium on Chemical Bonding (CBOND2022) — Efficiency and Suitability when Exploring the Conformational Space of Phase-Transfer Catalysts

Best poster Jan 2020
WATOC 2020 — Efficiency and Suitability when Exploring the Conformational Space of Phase-Transfer Catalysts

Best flash talk Jan 2020
Institute of Chemistry of Ireland Postgraduate Chemistry Research Symposium — Anion Recognition by Neutral and Cationic Iodotriazole Halogen Bonding Scaffolds

SFI fellowship for Ph.D. studies Jan 2019
Science Foundation Ireland

UAM–Fujitsu fellowship for TCCM master's studies Jan 2016
Universidad Autónoma de Madrid / Fujitsu