Andrea Darù

Chicago (IL, USA)
andrea.daru.89@gmail.com; adaru@uchicago.edu
Citizenship: Italian

LinkedIn
Google Scholar
0000-0002-0825-2101
Personal Website

Working experience

19 Dec 2022 - present **Postdoctoral Researcher** - University of Chicago (Chicago, IL)
Field Computational chemistry applied to solid state catalysis, metal- and covalent- organic frameworks properties and structural prediction, water and gas adsorption on solids
PI Prof. Laura Gagliardi

20 Oct '20 - 16 Dec '22 **Postdoctoral Associate** - Scripps Research (San Diego, CA)
Field Computational chemistry and kinetic studies applied to metal catalysis and origin of life processes
PI Prof. Donna Blackmond

Jan - Feb 2018 **Visiting PhD Student** - Syngenta (Stein, CH)
Project Reactivity study with Fukui functions as molecular descriptors for ML database

Education

21 Feb 2020 **PhD Marie Skłodowska-Curie Fellow** - KU Leuven (Belgium)
Thesis title Non-noble metal catalysis for cross-coupling reactions: computational insights
Project NoNoMeCat: Non-Noble Metal Catalysis Horizon2020
Supervisors Prof. Jeremy N. Harvey, Prof. Xile Hu [EPFL]

17 Dec 2015 **Postgraduate Degree** - University of Zaragoza (Spain)
Subjects Organic Synthesis, Computational Chemistry
Supervisors Prof. Pedro Merino, Prof. Tomas Tejero

12 Dec 2013 **MSc Degree in Chemical Science** - University of Ferrara (Italy)
Thesis title Synthesis of self-concentrating biocides as polymeric additives
Supervisors Prof. Marco Fogagnolo, Dr. Giancarlo Fantin

16 Dec 2011 **BSc Degree in Chemistry** - University of Ferrara (Italy)
Thesis title Strategies for conjugation of oligonucleotides
Supervisor Prof. Alessandro Massi

Academic experience

1-3 Nov 2021 **Virtual Simons Collaboration on the Origin of Life Annual Symposium**
Poster: Computational insights into the origin of stereoselectivity of the Strecker reaction

14 Jun 2019 **NoNoMeCat Symposium** - Syngenta (Stein - CH)
Poster: Computational Study of Nickel-catalysed Negishi Arylation of Propargylic bromides

04 Jun 2019 **VSC User Day** - Brussels (BE)
Poster: Computational Study of Nickel-catalysed Negishi Arylation of Propargylic Bromides

19 May 2019 **Open Day KU Leuven - Discovering chemistry & life sciences**
Task: Organizer for the Quantum Chemistry division

8–11 Jul 2018 **ECIRM: European Colloquium on Inorganic Reaction Mechanisms** - Barcelona (ES)
Talk: Computational Study of Olefin Reductive Coupling Reaction Catalyzed by Iron Bromide

13–15 Jun 2018 **Computational Catalysis for Sustainable Chemistry** - Tarragona (ES)
Poster: Computational Study of Nickel-catalysed Negishi Arylation of Propargylic Bromides

22 May 2018 **VSC User Day** - Brussels (BE)
Poster & Talk: Computational Expenses of Inorganic Computational Chemistry Calculations

17–20 Jul 2018 **EJD-TCCM Conference** - Leuven (BE)
Task: Web designing and management of participants

30 Jan 2018 **QCB13: Quantum Chemistry in Belgium** - Brussels (BE)

Poster: Computational Study of Olefin Reductive Coupling Reaction Catalyzed by Iron Bromide

02 Jun 2017 **VSC User Day** - Brussels (BE)

Poster: Computational Study of Olefin Reductive Coupling Reaction Catalyzed by Iron Bromide

20 May 2017 **Open Day of KU Leuven - 200 years advanced curiosity**

Task: Organizer for the Quantum Chemistry division

19—22 March 2017 **CMS Conference** - University of Warwick (UK)

Poster: Computational Study of Olefin Reductive Coupling Reaction Catalyzed by Iron Bromide

Computer skills

Coding	Bash, Python (ASE, RDKit, NumPy, Pandas)
OS	Linux, Windows, Android
DRMS - HPC	Torque, Slurm
Chemistry	Gaussian, Molpro, ORCA, VASP, Turbomole, NAMD

Editorial Experience

Currently active peer reviewer for Journal of Organic Chemistry, and ACS Catalysis.

Languages skills

Mother tongue	Italian
Foreign languages	English (Fluent), Spanish (Fluent)

Teaching activity

2^{nd} semester 2019 **Stuctural Bioinformatics Exercise** - KU Leuven (BE)

Task: Assistant of Prof. Harvey for practical exercise part

a.y. 2017/2018 **Master Thesis Supervision** - KU Leuven (BE)

Title: Computational study of the mechanism of the triazolization reaction

Jan 2017 **Workshop: Introduction to Computational Chemistry** - KU Leuven (BE)

Task: Teaching and exercise to PhD students of the NoNoMeCat network

Publications

(under revision) **Darù, A.***; Harvey, J. N. Computational Exploration of Nickel-catalysed Negishi Arylation of Propargylic Bromides.

(under revision) Kurandina, D.; Huang, B.; Xu, W.; Hanikel, N.; **Darù, A.**; Stroscio, G. D.; Wang, K.; Gagliardi, L.; Toste, F. D.; Yaghi O. M. Porous Crystalline Nitrone-Linked Covalent Organic Framework.

13 de Gombert, A.; **Darù, A.**; Ahmed, T. S.; Haibach, M. C.; Li-Matsuura, R.; Young, C.; Henry, R. F.; Cook, S. P.*; Shekhar, S.*; Blackmond, D. G.* Mechanistic Insight into Cu-Catalyzed C-N Coupling of Hindered Aryl Iodides and Anilines Using a Pyrrol-ol Ligand Enables Development of Mild and Homogeneous Reaction Conditions. *ACS Cat.* **2023**.

12 **Darù, A.***; Martín-Fernández, C.; Harvey, J. N. Iron-catalyzed Kumada Cross-coupling Reaction Involving $Fe_8Me_{12}^-$ and Related Clusters: A Computational Study. *ACS Cat.* **2022**, 12, 12678-12688.

11 Hao, W.; Joe, C. L.; **Darù, A.**; Ayers, S.; Ramirez, A.; Sandhu, B.; Daley, R.A.; Chen, J. S.; Schmidt, M. A.*; Blackmond, D. G.* Kinetic and Thermodynamic Considerations in the Rh-Catalyzed Enantioselective Hydrogenation of 2-Pyridyl-Substituted Alkenes. *ACS Cat.* **2022**, 12, 59615969.

10 Hao, W.; Joe, C. L.; Ayers, S.; **Darù, A.**; Daley, R. A.; Domanski, M.; Chen, J. S.; Schmidt, M. A.*; Blackmond, D. G.* Ru-Catalyzed Enantioselective Hydrogenation of 2-Pyridyl Substituted Alkenes and Substrate-Mediated H/D Exchange. *ACS Cat.* **2022**, 12, 1150-1160.

9 Legnani, L.; **Darù, A.**; Jones, A. X.; Blackmond, D. G.* Mechanistic Insight Into the Origin of Stereoselectivity in the Ribose-Mediated Strecker Synthesis of Alanine. *J. Am. Chem. Soc.* **2021**, 143, 7852-7858.

8 Harvey, J. N.; **Darù, A.** Computational Chemistry and Non-noble Metal-catalyzed Cross-coupling Reaction Mechanisms. *Chimia* **2020**, 74, 467-469.

7 PérezGarcía, P. M.#; **Darù, A.#**; Scheerder, A. R.; Lutz, M.; Harvey, J. N.*; Moret, M-E.* Oxidative Addition of Aryl Halides to a Triphosphine Ni(0) Center to Form Pentacoordinate Ni(II) Aryl Species. *Organometallics* **2020**, 39, 1139-1144.

6 Ploeger, M. L.#; **Darù, A.#**; Harvey, J. N.*; Hu, X.* Reductive Cleavage of Azoarene as a Key Step in Nickel-Catalyzed Amidation of Esters with Nitroarenes. *ACS Cat.* **2020**, 10, 2845-2854.

5 **Darù, A.**; Hu, X.*; Harvey, J. N.* Iron-Catalyzed Reductive Coupling of Alkyl Iodides with Alkynes to Yield Cis-Olefins: Mechanistics Insights from Computation. *ACS Omega* **2019**, 5, 1586-1594.

4 Ríos-Gutiérrez, M.; **Darù, A.**; Tejero, T.; Domingo, L. R.; Merino, P.* A Molecular Electron Density Theory Study of the [3 + 2] Cycloaddition Reaction of Nitrones With Ketenes. *Org. Biomol. Chem.* **2017**, 15, 1618-1627.

3 Roca-López, D.; **Darù, A.**; Tejero, T.; Merino, P.* Revisiting Oxime-Nitrone Tautomerism. Evidences of Nitrone Tautomer Participation in Oxime Nucleophilic Addition Reactions. *RSC Adv.* **2016**, 6, 22161-22173.

2 **Darù, A.**; Roca-López, D.; Tejero, T.; Merino, P.* Revealing Stepwise Mechanisms in Dipolar Cycloaddition Reactions: Computational and Topological Study of the Reaction between Nitrones and Isocyanates *J. Org. Chem.* **2016**, 81, 673-680.

1 Matute, R.; García-Viñuales, S.; Hayes, H.; Ghirardello, M.; **Darù, A.**; Tejero, T.; Delso, I.; Merino, P.* Recent Advances in the Preparation of Enantiomerically Pure Hydroxylamines from Nitrones. *Curr. Org. Synth.* **2016**, 13, 669-686.

References

PI PostDoc 1 Prof. Donna G. Blackmond, Scripps Research (San Diego, CA)
Email: blackmon@scripps.edu - Telephone: +1 (858) 784-2197
`https://www.scripps.edu/blackmond/index.html`

PhD supervisor Prof. Jeremy Harvey, KU Leuven (Belgium)
Email: jeremy.harvey@kuleuven.be - Telephone: +32 16372198
`https://jeremyharveygroup.wordpress.com/`

Postgrad supervisor Prof. Pedro Merino, University of Zaragoza (Spain)
Email: pmerino@unizar.es - Telephone: +34 876 553783
`www.bioorganica.es`