

José Augusto Berrocal



I am an organic chemist with a broad interest in supramolecular systems and stimuli-responsive molecules and materials. Our group is active in the design, synthesis, and characterization of materials that are potentially applicable to sustainable development.

ORCID ID 0000-0003-3435-8310

Researcher ID AAK-3176-2021

WORK EXPERIENCE

- 07/2023 - present** Group Leader (Tenure track position)
Institute of Chemical Research of Catalonia (ICIQ) (Tarragona, Spain)
- Maître Assistant (Non-tenure track position; 10% appointment)
Adolphe Merkle Institute (AMI) at University of Fribourg (Switzerland)
- 09/2019 - 06/2023** Maître Assistant (Non-tenure track position; 100% appointment)
Adolphe Merkle Institute (AMI) at University of Fribourg (Switzerland)
- 09/2017 - 09/2019** Postdoctoral Researcher in the group of Prof. Ben L. Feringa
Rijksuniversiteit Groningen (RUG) (the Netherlands)
- 04/2014 - 08/2017** Postdoctoral Researcher in the group of Prof. E. W. "Bert" Meijer
Eindhoven University of Technology (TU/e) (the Netherlands)
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EDUCATION

- 10/2010 - 01/2014** PhD in Chemical Sciences (Awarded on January 10th, 2014)
University "La Sapienza", Rome (Italy)
PhD Advisors: Profs. Luigi Mandolini and Stefano Di Stefano
Thesis title: "Quantitative features of intramolecular reactions"
- 11/2012 - 05/2013** Visiting PhD student in the group of Prof. E. W. "Bert" Meijer
Eindhoven University of Technology (TU/e) (the Netherlands)
- 10/2008 - 07/2010** M.Sc. in Chemistry
University "La Sapienza", Rome (Italy)
Mark: 110/110 cum laude
Thesis title: "Studies on macrocyclization systems under thermodynamic control"
- 10/2005 - 09/2008** B.Sc. in Chemistry
University "La Sapienza", Rome (Italy)
Mark: 110/110 cum laude
Thesis title: "Synthesis and properties of a new family of cyclophane formaldehyde acetals"

TEACHING EXPERIENCE AND OUTREACH ACTIVITIES

- 05/2022 - 06/2023** KidsUni
Hands-on experience with polymer chemistry for primary school students
Adolphe Merkle Institute (AMI)
- 09/2021 - 06/2023** Course Co-Responsible – Selected Topics in Organic Chemistry
Chemistry Department, University of Fribourg (Switzerland)
- 09/2020 - 06/2023** Course Co-Responsible – Functional Materials
Chemistry Department, University of Fribourg (Switzerland)
- 09/2020 - 06/2023** Practical Course Co-Organizer and Teacher – Basic Lab Skills
Chemistry Department, University of Fribourg (Switzerland)
- 04/2014 - 08/2017** Co-Lecturer – Practical Organic Chemistry and Materials (OGO project)
Department of Chemistry and Chemical Engineering, TU/e (the Netherlands)
- 10/2011 - 09/2013** Students' Tutor for Organic Chemistry (competitive selection process)
Department of Chemistry, University "La Sapienza", Rome (Italy)
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SUPERVISION AND COACHING

- 01/2019 - present** Supervision of: 3 postdocs (Dr. Visuta Engkagul, Dr. James Hemmer, Dr. Justus Wesseler)
5 PhD students (Ilaria Onori, Matilde Folkesson, Irene Antignano (visiting),
Lorenzo Paleari (visiting), Youwei Ma (visiting))
3 M. Sc. students (Marco Caliari, Pacifique Umubyeyi, Kjell Cornelis)
Adolphe Merkle Institute (AMI)
- 04/2014 - 08/2017** Coach to: 3 M. Sc. students (Rob van Geffen, Mark Gosens, Alex Huizinga)
1 B. Sc. student (Kiyam Oroudji)
Department of Chemistry and Chemical Engineering, TU/e (the Netherlands)
- 10/2010 - 01/2014** Coach to: 3 M. Sc. students (Marzia Galli, Federica Laurenzi, Simone Albano)
2 B. Sc. students (Augusto Fantozzi, Valeria D'Amico)
Department of Chemistry, University "La Sapienza", Rome (Italy)
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INSTITUTIONAL RESPONSIBILITIES

- 09/2022 - 06/2023** Responsible for the organization of the institute seminars
Adolphe Merkle Institute (AMI)
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MEMBERSHIP OF SCIENTIFIC SOCIETIES

- 2019 - present** American Chemical Society (ACS)
- 2019 - present** Swiss Chemical Society (SCS)
- 2010 - present** Italian Chemical Society (SCI)

REVIEWING ACTIVITIES

2021 - present	Reviewer for ACS journals " <i>Journal of the American Chemical Society</i> ", " <i>ACS Macro Letters</i> ", " <i>Macromolecules</i> ", and " <i>ACS Polymer Au</i> "
2021 - present	Reviewer for Elsevier journals " <i>European Polymer Journal</i> ", " <i>Chemosphere</i> ", and " <i>Materials Chemistry and Physics</i> "
2018 - present	Reviewer for RSC journals " <i>Chemical Communications</i> ", " <i>Dalton Transactions</i> ", " <i>Chemical Science</i> ", and " <i>New Journal of Chemistry</i> "
2016 - present	Reviewer for Wiley journals " <i>Chemistry - A European Journal</i> ", and " <i>Journal of Polymer Science - Part A</i> "

COMMITTEES OF TRUST

2023	Member of the PhD thesis reading committee of Edgar Fuentes (<i>Institute of Bioengineering of Catalonia</i>), Lorenzo Paleari (<i>University of Rome "Tor Vergata"</i>), and Daniele Del Giudice (<i>University of Rome "La Sapienza"</i>) Member of the PhD committee of Ankita Mandal (<i>University of Fribourg; PhD defense tentatively scheduled for April 2023</i>) Member of the PhD committees of Nicola Camedda, Federica Cester Bonati, and Carlo Vezzoni (<i>University of Parma; PhD defenses scheduled for May 18th, 2023</i>)
2022	Member of the PhD committee of Dr. Livius Muff (<i>Adolphe Merkle Institute</i>)
2021	Member of the PhD committee of Dr. Baptiste Monney (<i>Adolphe Merkle Institute</i>)
2020	Member of the PhD committee of Dr. Sergio Jurado (<i>Universitat Autònoma de Barcelona</i>) Member of the PhD thesis reading committee of Dr. Angelo Nicosia (<i>University of Catania</i>)

PARTICIPATION TO CONFERENCES AND INVITED TALKS

Conferences	Participation to 50+ international conferences, including (selected list) <i>Gordon Conference on Self-Assembly 2023</i> (poster) <i>ACS Fall Meeting 2022</i> (Chicago, oral) <i>ACS Spring Meeting 2020</i> (Philadelphia, oral online) <i>Gordon Conference on Self-Assembly 2019</i> (poster) <i>Frontiers in Chemistry 2018</i> (Yerevan (Armenia), oral)
Invited talks	<i>Swiss Academy of Sciences - Young Faculty Meeting 2023</i> (Griesalp, May 31 st -June 1 st) <i>University of Geneve</i> (January 26 th , 2023) <i>POLYMAT</i> (San Sebastian, September 2 nd , 2022) <i>University of Bern</i> (June 29 th , 2021) <i>BASF</i> (Ludwigshafen, June 20 th 2018)

ORGANIZATION OF CONFERENCES

22-24/03/2023	Dynamic Materials, Crystals and Phenomena Conference (DynaMIC23) URL: https://www.nanoge.org/DynaMIC23/home <i>Adolphe Merkle Institute, University of Fribourg (Switzerland)</i> Role: Local Coordinator
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FELLOWSHIPS, GRANTS AND AWARDS

- 01/2023** Thieme Chemistry Journals Award 2023
- 07/2023 - 06/2028** Funding agency: European Research Council (ERC) Starting Grant 2021
Project title: *Reversible Heterolytic Mechanophores for Dynamic Bulk Materials (ReHuse)*
Funding amount: 1.5M€
Role: Primary Investigator (PI)
Success rate <10%
- 06/2022 - 05/2025** Funding agency: Office of Naval Research (ONR) Global
Project title: *Mechanochromic Polyurethane Materials Comprising Triarylmethane Mechanophores*
Funding amount: 500k€
Role: PI
- 06/2022 - 05/2026** Funding agency: European Innovation Council (EIC) Pathfinder Grant
Project title: *Biointegrable soft actuators alimented by metabolic energy (INTEGRATE)*
Funding amount: 3 M€ in total, 1.3 M€ for Berrocal and another PI from AMI
Role: Co-Lead of the Consortium; One of the PIs of the Consortium and Work Package (WP) leader
Success rate 6%
- 06/2022** Best Keynote Presentation
Symposium for Young Chemists (SYNC) 2002: Innovation and Sustainability
Rome (Italy), June 20-23
- 04/2021 - 04/2022** Funding agency: Swiss National Science Foundation (Spark project)
Project title: *Stimuli-induced proton shuttling – new concepts for new energy harvesting materials*
Funding amount: 100 kCHF
Role: PI
Success rate ~10%
- 10/2020 - 09/2021** Funding source: Climeworks (Industry)
Project title: *Polymers for carbon capture*
Funding: 150 kCHF
Role: Co-PI
- 2012** “Avvio alla Ricerca” competitive fellowship
University of Rome “La Sapienza”
- 2010 - 2013** Competitive PhD scholarship
Department of Chemistry, University of Rome “La Sapienza”
- 2008** Selected for the Roche Continents 2008
<https://www.roche.com/about/philanthropy/arts-and-culture/roche-continents/>
Salzburg, Austria
100 students selected per year

LIST OF PUBLICATIONS (as of August 1st, 2023)

1. Closed-loop recycling of vinylogous urethane vitrimers
Ma, Y.; Jiang, X.; Yin, J.; Shi, Z.*; **Berrocal, J. A.***; Weder, C.*
Angew. Chem. Int. Ed. Engl. 2023, e202306188
2. Sustainable phase change materials (PCMs): waste fat from cooking pork meat confined in polypropylene fibrous mat from waste surgical mask and porous bio-silica
Bragaglia, M.; Lamastra, F. M.; **Berrocal, J. A.**; Paleari, L.; Nanni, F.
Materials Today Sustainability 2023, 100454
3. An electrolyte additive for the improved high voltage performance of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO) cathode in Li-ion batteries
Nguyen, M. T.; Pham, H. Q.; **Berrocal, J. A.**; Gunkel, I.; Steiner, U.
J. Mat. Chem. A 2023, 11, 7670-7678
4. Towards eco-sustainable rubber compounds: the use of waste raw materials
Bragaglia, M.; Paleari, L.; **Berrocal, J. A.**; Lamastra, F. R.; Nanni, F.
J. Appl. Pol. Sci. 2023, 140, e53750
5. Computational Design of Anisotropic Nanocomposite Actuators
Ianiro, A.; **Berrocal, J. A.**; Tuinier, R.; Mayer, M.; Weder, C.
J. Chem. Phys. 2023, 158, 014901
6. Chemical Upcycling of Conventional Polyureas into Dynamic Covalent Poly(aminoketoenamides)
Ma, Y.; Jiang, X.; Yin, J.; Weder, C.*; **Berrocal, J. A.***; Shi, Z.*
Angew. Chem. Int. Ed. Engl. 2023, e202212870 (Highlighted in ChemistryViews as "Cost-Efficient Upcycling of Polyurea Waste")
7. Supramolecular Stability of Benzene-1,3,5-tricarboxamide Supramolecular Polymers in Biological Media: beyond the Stability-Responsiveness Trade-off
Fuentes, E.; Gabaldón, Y.; Collado, M.; Dhiman, S.; **Berrocal, J. A.**; Pujals, S.; Albertazzi, L.
J. Am. Chem. Soc. 2022, 144, 21196-21205
8. A Perspective on the Force-Induced Heterolytic Bond Cleavage in Triarylmethane Mechanophores
Hemmer, J. R.; **Berrocal, J. A.***
Synlett 2022, 33, 1681-1687
9. Polyaromatic Cores for the Exfoliation of Popular 2D Materials
Garrido, M.; Barrejón, M.; **Berrocal, J. A.**; Syrgiannis, Z.; Prato, M.
Nanoscale 2022, 14, 8986-8994
10. Strain-Correlated Mechanochromism in Different Polyurethanes Featuring a Supramolecular Mechanophore
Traeger, H.; Sagara, Y.; **Berrocal, J. A.**; Schrettl, S.; Weder, C.
Polym. Chem. 2022, 13, 2860-2869
11. Tuning the Donor-Acceptor Interactions in Phase-Segregated Block Molecules
Lamers, B. A. G.; van Son, M. H. C.; de Graaf, F. V.; van den Bersselaar, B. W. L.; de Waal, B. F. M.; Komatsu, K.; Sato, H.; Aida, T.; **Berrocal, J. A.**; Palmans, A. R. A.; Vantomme, G.; Meskers, S. C. J.; Meijer, E. W.
Mater. Horiz., 2022, 9, 294-302
12. Heterolytic Bond Cleavage in a Scissile Triarylmethane Mechanophore
Hemmer, J. R.; Rader, C.; Wilts, B. D.; Weder, C.*; **Berrocal, J. A.***
J. Am. Chem. Soc. 2021, 143, 18859-18863 (Highlighted as "JACS Spotlight" 2021, 143, 19241-19242)
13. Discordant Supramolecular Fibres Reversibly Depolymerised by Temperature and Light
Gerth, M.; **Berrocal, J. A.**; Bochicchio, D.; Pavan, G. M.; Voets, I. K.
Chem. Eur. J. 2021, 27, 1829-1838
14. Stepwise Adsorption of Alkoxy-Pyrene Derivatives onto a Lamellar, Non-Porous Naphthalenediimide-Template on HOPG
Heideman, G. H.[§]; **Berrocal, J. A.[§]**; Stöhr, M.; Meijer, E. W.; Feringa, B. L.
Chem. Eur. J. 2021, 27, 207-211
15. Tuning of Morphology by Chirality in Self-Assembled Structures of Bis (Urea) Amphiphiles in Water
Tosi, F.; **Berrocal, J. A.**; Stuart, M. C. A.; Wezenberg, S. J.; Feringa, B. L.
Chem. Eur. J. 2021, 27, 326-330
16. Combinatorial Selection Among Geometrical Isomers of Discrete Long Carbon Chain-Naphthalenediimides Induces Local Order at the Liquid/Solid Interface
Berrocal, J. A.[§]; Heideman, G. H.[§]; de Waal, B. F. M.; Meijer, E. W.; Feringa, B. L.
ACS Nano 2020, 14, 13865-13875

17. Molecular Motor-Functionalized Porphyrin Cage Compounds
Gilissen, P. J.; White, P. B.; **Berrocal, J. A.**; Vanthuyne, N.; Rutjes, F. P. J. T.; Feringa, B. L.; Elemans, J. A. W. W.; Nolte, R.
Nat Commun. 2020, 11, 5291
18. Synthesis of Core-Modified Third-Generation Light-Driven Molecular Motors
Berrocal, J. A.; Pfeifer, L.; Hejinen, D.; Feringa, B. L.
J. Org. Chem. 2020, 85, 16, 10670–10680
19. An Azobenzene-Based Single-Component Supramolecular Polymer Responsive to Multiple Stimuli in Water
Fuentes, E.; Gerth, M.; **Berrocal, J. A.**; Matera, C.; Gorostiza, P.; Voets, I. K.; Pujals, S.; Albertazzi, L.
J. Am. Chem. Soc. 2020, 142, 22, 10069–10078
20. Engineering Long-Range Order in Supramolecular Assemblies on Surfaces: The Paramount Role of Internal Double Bonds in Discrete Long-Chain Naphthalenediimides
Berrocal, J. A.[§]; Heideman, G. H.[§]; de Waal, B. F. M.; Enache, M.; Havenith, R. W. A.; Stöhr, M.; Meijer, E. W.; Feringa, B. L.
J. Am. Chem. Soc. 2020, 142, 4070–4078
21. Tandem Catalysis in Multicomponent Solvent-Free Biofluids
Atkins, D. L.; **Berrocal, J. A.**; Mason, A. F.; Voets, I. K.
Nanoscale 2019, 11, 19797–19805
22. Directing the Solid-State Organization of Racemates via Structural Mutation and Solution-State Assembly Processes
Kulkarni, C.; **Berrocal, J. A.**; Lutz, M.; Palmans, A. R. A.; Meijer, E. W.
J. Am. Chem. Soc. 2019, 141, 6302–6309
23. Selenoamides modulate dipole-dipole interactions in hydrogen bonded supramolecular polymers of 1,3,5-substituted benzenes
Berrocal, J. A.[§]; Mabesoone, M. F. J.[§]; García-Iglesias, M.; Huizinga, A.; Meijer, E. W.; Palmans, A. R. A.
Chem. Commun. 2019, 55, 14906–14909
24. Resistive switching in an organic supramolecular semiconducting ferroelectric
Casellas, N. M.; Urbanaviciute, I.; Cornelissen, T. D.; **Berrocal, J. A.**; Torres, T.; Kemerink, M.; García-Iglesias, M.
Chem. Commun. 2019, 55, 8828–8831
25. Inherently Chiral Cone-Calix[4]Arenes via a Subsequent Upper Rim Ring-Closing/Opening Methodology
Berrocal, J. A.^{*}; Baker, M. B.; Baldini, L.; Casnati, A.; Di Stefano, S.
Org. Biomol. Chem. 2018, 16, 7255–7264
26. Supramolecular Loop Stitches of Discrete Block Molecules on Graphite: Tunable Hydrophobicity by Naphthalenediimide End-Capped Oligodimethylsiloxane
Berrocal, J. A.; Teyssandier, J.; Goor, O. J. G. M.; De Feyter, S.; Meijer, E. W.
Chem. Mater. 2018, 30, 3372–3378
27. Peptide-Driven Charge-Transfer Organogels Built from Synergetic Hydrogen Bonding and Pyrene-Naphthalenediimide Donor-Acceptor Interactions
Bartocci, S.; **Berrocal, J. A.**^{*}; Guarracino, P.; Grillaud, M.; Franco, L.^{*}; Mba, M.^{*}
Chem. Eur. J. 2018, 24, 2920–2928
28. Photoswitchable Nanomaterials Based on Hierarchically Organized Siloxane Oligomers
Zha, R. H.; Vantomme, G.; **Berrocal, J. A.**; Gosens, R. P. J.; De Waal, B. F. M.; Meskers, S.; Meijer, E. W.
Adv. Funct. Mater. 2018, 28, 1703952
29. Variations in the Fuel Structure Control the Rate of the Back and Forth Motions of a Chemically Fuelled Molecular Switch
Biagini, C.; Albano, S.; Caruso, R.; Mandolini, L.; **Berrocal, J. A.**; Di Stefano, S.
Chem. Sci. 2018, 9, 181–188
30. Supramolecular Polymerization of a Ureidopyrimidinone-Based [2]Catenane Prepared via Ring-Closing Metathesis
Teunissen, A. J. P.[§]; **Berrocal, J. A.**[§]; Corbet, C. H. W. A.; Meijer, E. W.
J. Polym. Sci. Part A: Polym. Chem. 2017, 55, 2971–2976
31. Unraveling the Driving Forces in the Self-Assembly of Monodisperse Naphthalenediimide-Oligodimethylsiloxane Block Molecules
Berrocal, J. A.; Zha, R. H.; De Waal, B. F. M.; Lugger, J. A. M.; Lutz, M.; Meijer, E. W.
ACS Nano 2017, 11, 3733–3741 (Highlighted in *Nature Nanotechnology* <https://doi.org/10.1038/nnano.2017.93>)
32. Influence of Topology on the Gelation Behavior of Coordination Polymers Prepared via ROMP of Macrocyclic Olefins
Albano, S.; Fantozzi, A.; **Berrocal, J. A.**; Di Stefano, S.
J. Polym. Sci. Part A: Polym. Chem. 2017, 53, 1237–1242

33. Highly Circularly Polarized Broad-Band Emission from Chiral Naphthalene Diimide-Based Supramolecular Aggregates
Salerno, F.; **Berrocal, J. A.**; Haedler, A. T.; Zinna, F.; Meijer, E. W.; Di Bari, L.
J. Mat. Chem. C 2017, 5, 3609-3615
34. Mesoscopic Helical Architectures via Self-Assembly of Porphyrin-Based Discotic Systems
Vela, S.[§]; **Berrocal, J. A.**[§]; Atienza, C.; Meijer, E. W.; Martin, N.
Chem. Commun. 2017, 53, 4084-4087
35. Coupling of the Decarboxylation of 2-Cyano-2-phenylpropanoic Acid to Large-Amplitude Motions: a Convenient Fuel for an Acid-Base-Operated Molecular Switch
Berrocal, J. A.; Biagini, C.; Mandolini, L.; Di Stefano, S.
Angew. Chem. Int. Ed. Engl. 2016, 24, 6997-7001
36. Consequences of Conformational Flexibility in Hydrogen-Bond-Driven Self-Assembly Processes
Berrocal, J. A.[§]; Di Meo, F.[§]; García-Iglesias, M.[§]; Gosens, R. P. J.; Meijer, E. W.; Linares, M.; Palmans, A. R. A.
Chem. Commun. 2016, 52, 10870-10873
37. A Cu^I-Based Metallo-Supramolecular Gel-Like Material Built from a Library of Oligomeric Ligands Featuring Exotopic 1,10-Phenanthroline Units
Berrocal, J. A.; Albano, S.; Mandolini, L.; Di Stefano, S.
Eur. J. Org. Chem. 2015, 34, 7504-7510
38. Ring-Opening Metathesis Polymerization of a Diolefinic [2]-Catenane-Copper(I) Complex: an Easy Route to Polycatenanes
Berrocal, J. A.; Pitet, L.; Nieuwenhuizen, M.M.L.; Mandolini, L.; Meijer, E.W.; Di Stefano, S.
Macromolecules 2015, 48, 1358-1363
39. Copper-Induced Amplification of a [2]Catenane in a Virtual Dynamic Library of Macrocyclic Alkenes
Berrocal, J. A.; Nieuwenhuizen, M.M.L.; Mandolini, L.; Meijer, E.W.; Di Stefano, S.
Org. Biomol. Chem. 2014, 12, 6167-6174
40. Highly Efficient Intramolecular Cannizzaro Reaction between 1,3-Distal Formyl Groups at the Upper Rim of a Cone-Calix[4]arene
Galli, M.; **Berrocal, J. A.**; Di Stefano, S.; Cacciapaglia, R.; Mandolini, L.; Baldini, L.; Casnati, A.; Ugozzoli, F.
Org. Biomol. Chem. 2012, 10, 5109-5112
41. Target-Induced Amplification in a Dynamic Library of Macrocycles. A Quantitative Study
Berrocal, J. A.; Cacciapaglia, R.; Di Stefano, S.; Mandolini, L.
New J. Chem. 2012, 36, 40-43
42. A Well-Behaved Dynamic Library of Cyclophane Formaldehyde Acetals Incorporating Diphenylmethane Units
Berrocal, J. A.; Cacciapaglia, R.; Di Stefano, S.
Org. Biomol. Chem. 2011, 9, 8190-8194

[§] Equal contribution from these authors

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