

## **Carles E. Curutchet**

Carles E. Curutchet is Serra Húnter Full Professor at the University of Barcelona, where he graduated in Chemistry and got his PhD, and serves as Director of the Department of Pharmacy, Pharmaceutical Technology and Physical Chemistry. He founded the Computational Photobiology Lab in 2012 as a Ramón y Cajal researcher, later promoted to Serra Húnter Associate Professor (2016) and Full Professor (2020), having spent postdoctoral periods in Italy (Univ. of Pisa and Parma) and Canada (Univ. of Toronto). He is a collaborator of the leading software in Quantum Chemistry Gaussian (USA), has published 79 articles (4025 citations, h-index 38, WoS), and is a regular reviewer for journals (>100 articles) and agencies (50 projects from 13 different agencies since 2012). He has given 14 invited lectures including 4 courses in international schools, and since 2012 has been funded through 4 national projects, a regional Industrial Doctorate and the European ALLODD H2020-MSCA-ITN-2020 network.

## **Anna Masdeu**

Catedràtica d'universitat amb 34 anys d'experiència en la Docència en Química General i Química Inorgànica a nivell de grau, màster i doctorat (13 tesis dirigides). Expertesa en recerca en aspectes en catalisi relacionats amb l'activació de diòxid de carboni i reaccions de carbonilació amb especial focus en l'ús de solvents verds. Resultats publicats en 90 publicacions en revistes interacionals (h-index 28). Participació en el Màster de Formació de Professorat de Secundària, Idiomes i Formació professional (2012-actual) i en activitats de Divulgació (Distinció Jaume Vicens Vives a la qualitat docent universitària en la modalitat col·lectiva amb el project "Repte experimenta a l'aula: potenciant les habilitats suaus en un entorn STEAM", 2023).

## **Laura Masgrau**

La Dr. Laura Masgrau és professora agregada al Departament de Química Física de la Universitat Autònoma de Barcelona (UAB). És experta en modelització molecular de sistemes biomoleculars, particularment en mètodes de mecànica quàntica-mecànica molecular, docking proteïna-ligand i simulacions de dinàmica molecular. Llicenciada (1997) i doctora (2002) en Química per la UAB, va fer postdoctorats a la Universitat de Leicester (Regne Unit) i a l'Institut Pasteur de París i va tornar a la UAB com a investigadora Ramón y Cajal, on va iniciar la seva pròpia línia de recerca. Ha sigut

secretària de l'Institut de Biotecnologia i Biomedicina de la UAB, ha tingut un contracte Talent a la UAB i ha sigut investigadora a ZYMVOL Biomodeling. El 2015 va ser guardonada amb una borsa de recerca de L'Oréal-UNESCO For Women in Science. Actualment, és la investigadora principal de dos projectes de recerca. Imparteix classes en diverses titulacions i màsters. És coautora d'unes 60 publicacions, ha supervisat 6 tesis doctorals (1 en curs) així com treballs de final de grau i màster.

### **Mariona Sadupe**

Mariona Sodupe earned her Bachelor's degree in Chemistry from the Universitat Autònoma de Barcelona (UAB) in 1985 and completed her PhD in Chemistry at the same institution in 1990. She then undertook a postdoctoral fellowship (1990-1992) at NASA Ames Research Center in California, supported by a Fulbright Fellowship, working with Prof. C.W. Bauschlicher. In 1992, she returned to UAB as an Associate Professor and since 2008 she has been a Full Professor in the Department of Chemistry. She has been awarded the Distinction of the Generalitat of Catalunya for the Promotion of Research in 2001 and the ICREA Academia Award in 2011. She has coauthored over 200 papers in international journals.

Her research primarily focuses on the structure and reactivity of chemical systems through quantum chemical methods. Recent projects include the computational modeling of: i) complex metal cation-biomolecule systems, particularly their role in neurodegenerative diseases, ii) biomolecule adsorption and reactivity on silica-based surfaces, relevant to prebiotic chemistry, and iii) catalysis.

### **Nicolás Pazos**

Dr. Nicolas Pazos-Perez is an expert in colloidal chemistry and nanomaterials. His expertise includes synthesis, surface functionalization, and self-assembly of nanoparticles. His current research is focused on harnessing these materials for SERS-based detection systems. He holds a Chemistry degree from the Universidade de Vigo. Completed his Ph.D. as part of a Marie Curie Research Training Network, conducting his research between Spain and Germany. Afterward, he spent five years as a Postdoctoral Research Associate at the University of Bayreuth, Germany. In 2013, returned to Spain and became Senior Research Officer at Medcom Advance in Tarragona. The following year, he was awarded a Marie Curie Fellowship and joined the University Rovira i Virgili

(URV) in Tarragona. In 2016, he transitioned to Medcom Tech as a Senior Research Officer, before rejoining the URV in 2017 under the prestigious Ramón y Cajal program. Since 2022, held the position of Aggregated Professor in the Department of Physical and Inorganic Chemistry at the URV.

### **Vicent Moliner**

Degree in chemistry from the University of Valencia (1988). Doctor in Chemistry from the University Jaume I, 1993, under the supervision of J. Andrés. R & D Technician in FERRO ENAMEL Spain (1990-1992). Appointed by Jaume I University as Assistant Professor of Faculty, 1994 and Full Professor in 2009. After early stays with Orlando Tapia (Uppsala) and Jiri Krechl (Prague), post-doc as Official Researcher at the University of Bath (1996-1997) with Ian Williams. Other shorter stays at the Institut de Biologie Structurale, Grenoble (France) in the group of M. Field; Universidade Federal do Pará, (Brasil) in the group of C. N. Alves; and Université Pierre et Marie Curie. Paris VI (France) in the group of O. Parisel. Associate Professor at University Jaume I from 1998 to 2009. Visiting professor at Lodz University of Technology during the years 2009-2010, and David Parkin visiting professor at University of Bath during 2017.

The interest of V. Moliner during the last years focuses on the development of QM/MM methods and the study of enzymatic reactions. The development of such methods opened the possibility to study enzyme catalyzed reactions and applications such as the design of new biocatalysts or enzymatic inhibitors.