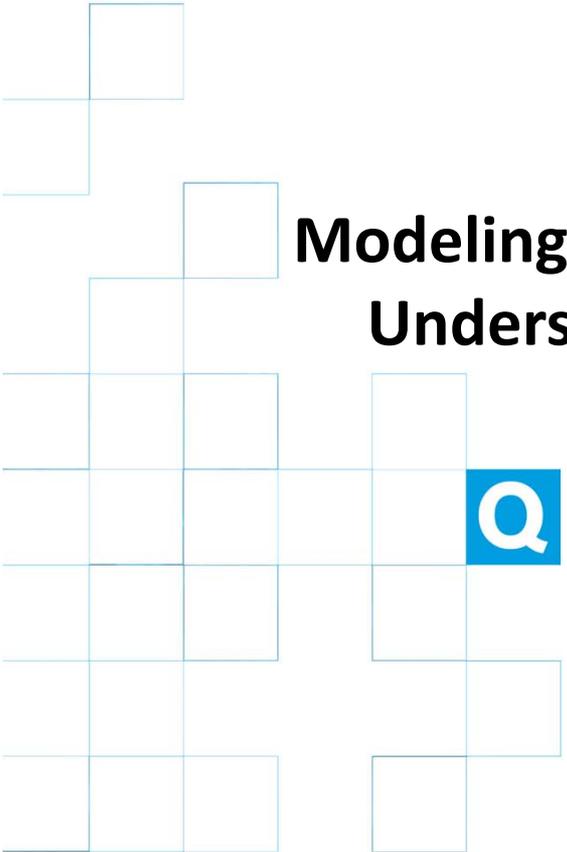


# CiQUS

Centro Singular de Investigación  
en Química Biológica e  
Materiais Moleculares

## Conferencia:

# Modeling Metal–Ligand Interfaces to Understand Selectivity in Catalysis



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## Manuel Ángel Ortuño

ICIQ, Catalonia, Spain

**13/02/2020**

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Aula de  
Seminarios do  
CIQUS  
**12:15h**

Más información:  
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## Biography

Dr. Manuel Ángel Ortuño was born and raised in Almería, where he did his bachelor's degree in Chemistry.

In 2014, he obtained his PhD at “Universitat Autònoma de Barcelona” under the supervision of Prof. Agustí Lledós and Prof. Gregori Ujaque.

In 2015, he started as postdoctoral associate at the University of Minnesota (USA) in the group of Prof. Christopher Cramer. During that time, he was also involved at management level in the “Inorganometallic Catalyst Design Center” directed by Prof. Laura Gagliardi.

In 2018, he joined the group of Prof. Núria López at “Institut Català d'Investigació Química” within the “Juan de la Cierva–Incorporación” programme. Since 2019, he holds a “Beatriu de Pinós” fellowship at the same institution.

He recently obtained 2 travel grants by HPC-Europa3 to access high-performance computing facilities and visit the University of Bonn in Germany.

His scientific profile focuses on the computational simulation of catalytic systems across different scales: from molecular organometallic chemistry to metal surfaces and porous materials.

Today he is going to present some research studies on how to “conciliate” homogeneous and heterogeneous catalysis.

## Title

Modeling Metal–Ligand Interfaces to Understand Selectivity in Catalysis

## Picture

