

Program

November 21st 2024

14:45-15:00 h	Welcome
15:00-15:30 h	Francesc Viñes “Environment Factors in Computational Catalysis”
15:30-16:00 h	Livia Giordano “From Supported Clusters to Single Atom Catalysts: Every Atom Counts”
16:00-16:30 h	Hans J. Freund “Model Systems in Heterogeneous Catalysis: Metal-Modified Silicate and Germanate Films”
16:30-17:30 h	Coffee break/Poster Session
17:30-18:00 h	Paul Bagus “Bonding and Interactions in UO_2^{2+} : Extracting Chemistry from Molecular Orbital Calculations”
18:00-18:30 h	Richard Catlow “Modelling Catalytic Processes for Sustainable Energy and Environment”
18:30-19:00 h	José A. Rodríguez “ C_1 Chemistry on Metal Carbide Systems: Boosting the Conversion of CO_2 and H_2 ”
19:00-22:00	Dinner/Poster Session

November 22st 2024

9:30-10:00	Marta Rendé “Red Española de Supercomputación”
10:00-10:30	Verónica Ganduglia-Pirovano “Challenging DFT: Unraveling CO Vibrations on Cerium Oxide Surfaces”
10:30-11:00	Alexander Shluger “Intrinsic Defects in Amorphous Oxides: Reality or Elusion?”
11:00-11:30	Josep M. Ricart “Exploring Catalysis on Metal Surfaces and Clusters with a Reactive Force Field”
11:30-12:00	Coffee break/Poster Session
12:00-12:30	Nino Russo “Problems and Perspectives in Computational Enzymatic Catalysis”
12:30-13:00	Paola Luches “Cerium Oxide: From Steady-State Surface Properties to Ultrafast Processes in Photoexcited States”
13:00-13:30	Konstantin M. Neyman “From CO on MgO to Catalytic Nanomaterials”
13:30-14:00	Honorees’ Address
14:00-16:00	Lunch courtesy of Francesc and Gianfranco