

# FIRST INTERNATIONAL SYMPOSIUM ON THE DFT MODELLING OF MATERIALS RELEVANT FOR WATER SPLITTING

## FRIDAY // 11 DEC. 2020 // PROGRAM

**9:00** | OPENING AND REMARKS  
FROM THE ACTION CHAIR

**SESSION 1, CHAIR:  
MICHELE PAVONE,**

UNIVERSITY OF NAPLES FEDERICO II, ITALY

**9:15**

**CARLO ADAMO** ▶ Development of quantum chemical methods for the description of the complex interfaces, Chimie, ParisTech

**10:05**

**MAYTAL CASPARY TOROKER** ▶ Material variations in nano-scaled nickel oxyhydroxide affecting the water oxidation reaction, Technion, Israel

**10:35**

**MARCOS FERNÁNDEZ GARCÍA** ▶ Hydrogen thermo-photo production using metal-promoted titania-based materials, ICP-CSIC, Spain

**11:05**

**KAI EXNER** ▶ Recent Advancements in the Theoretical Description of the Oxygen Evolution Reaction: Activity Descriptors and Screening Approaches, Duisburg-Essen Universität, Germany

**SESSION 2, CHAIR:**

**DOROTA RUTKOWSKA-ZBIK,**

URZY HABER INSTITUTE OF CATALYSIS AND  
SURFACE CHEMISTRY, KRAKOW, POLAND

**11:55**

**GIOVANNI DI LIBERTO** ▶ Theoretical Description of BiVO<sub>4</sub>-based Heterojunctions for Photocatalytic Water Splitting: Insights from DFT, Università degli Studi di Milano-Bicocca, Italy

**12:25**

**CHRISTIANA A. MITSOPOULOU** ▶ DFT Studies on the Mechanisms of Hydrogen Evolution Catalysed by Transition Metal Complexes, University of Athens, Greece

**12:55**

**YURI MASTRIKOV** ▶ Water adsorption on the stepped TiO<sub>2</sub>-terminated (001) SrTiO<sub>3</sub> surface, University of Latvia, Latvia

**13:25**

**QIUHUA LIANG** ▶ Monolayer Nitrides Doped with Transition Metals as Efficient Catalysts for Water Oxidation: The Singular Role of Nickel, Eindhoven University of Technology, The Netherlands

**13:55**

**ISKRA KOLEVA** ▶ DFT Modelling of Structure and Reducibility of Cerium Dioxide Nanoparticles Doped by Zirconium, University of Sofia "St. Kliment Ohridski", Bulgaria

**14:25**

CONCLUDING  
REMARKS

**12:25**

CONFERENCE  
CLOSING

LOCAL ORGANIZING  
COMMITTEE:

**Francesc Viñes, IQTCUB**  
**Konstantin Neyman, ICREA & IQTCUB**  
**Francesc Illas, IQTCUB**

NOTE:

The speakers are kindly requested to leave around 10 minutes for questions/comments