

# CA18234. Computational materials sciences for efficient water splitting with nanocrystals from abundant elements

## First International Symposium on the DFT Modelling of Materials Relevant for Water Splitting

Workshop of Working Group 1

Online meeting, December 11<sup>th</sup>, 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**, *Chimie, ParisTech*

Development of quantum chemical methods for the description of the complex interfaces

10:05 **Maytal Caspary Toroker**, *Technion, Israel*

Material variations in nano-scaled nickel oxyhydroxide affecting the water oxidation reaction

10:35 **Marcos Fernández García**, *ICP-CSIC, Spain*

Hydrogen thermo-photo production using metal-promoted titania-based materials

11:05 **Kai Exner**, *Duisburg-Essen Universität, Germany*

Recent Advancements in the Theoretical Description of the Oxygen Evolution Reaction: Activity Descriptors and Screening Approaches

11:35 Break

**Session 2, Chair: Dorota Rutkowska-Zbik**, *Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow, Poland*

11:55 **Giovanni di Liberto**, *Università degli Studi di Milano-Bicocca, Italy*

Theoretical Description of BiVO<sub>4</sub>-based Heterojunctions for Photocatalytic Water Splitting: Insights from DFT

12:25 **Christiana A. Mitsopoulou**, *University of Athens, Greece*

DFT Studies on the Mechanisms of Hydrogen Evolution Catalysed by Transition Metal Complexes

12.55 **Yuri Mastrikov**, *University of Latvia, Latvia*

Water adsorption on the stepped TiO<sub>2</sub>-terminated (001) SrTiO<sub>3</sub> surface

13:25 **Qiuhua Liang**, *Eindhoven University of Technology, The Netherlands*

Monolayer Nitrides Doped with Transition Metals as Efficient Catalysts for Water Oxidation: The Singular Role of Nickel

13:55 **Iskra Koleva**, *University of Sofia "St. Kliment Ohridski", Bulgaria*

DFT Modelling of Structure and Reducibility of Cerium Dioxide Nanoparticles Doped by Zirconium

14:25 Concluding remarks

14:35 Conference closing

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

Local organizing committee: Francesc Viñes, *IQTCUB*; Konstantin Neyman, *ICREA & IQTCUB*  
Francesc Illas, *IQTCUB*