

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

FRIDAY // 11 DEC. 2020 // PROGRAM

09:00 | OPENING AND REMARKS
FROM THE ACTION CHAIR

**SESSION 1, CHAIR:
MICHELE PAVONE**

UNIVERSITY OF NAPLES FEDERICO II, ITALY

09:15 | **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

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

11:55 | **GIOVANNI DI LIBERTO** ▶ Theoretical Description of BiVO₄-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 TiO₂-terminated (001) SrTiO₃ 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