International Conference on Computational Materials Science for Nanoscale Modelling

CA18234 Meeting in Naples

AULA CAIANIELLO - Department of Physics "Ettore Pancini" - University of Naples FEDERICO II

Complesso Universitario Monte Sant'Angelo - Via Cintia 21, 80126 Naples, ITALY

FEBRUARY 11-13, 2020

International Scientific Committee

Maytal Caspary Toroker - Technion, Israel

Michele Pavone - University of Naples Federico II, Italy

Francesc Illas - University of Barcelona, Spain

Nicolae Goga - Polytechnic of Bucharest, Romania

Sofia Calero - Universidad Pablo de Olavide, Spain

Anja Bieberle-Hütter - Dutch Institute for Fundamental Energy Research, Netherlands

Florian Libisch - Vienna University of Technology, Austria

Tomasz Wesolowski - University of Geneva, Switzerland

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Local Organizing Committee

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Scientific Secretariat

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SCIENTIFIC PROGRAM

Tuesday 11/02/2020

09:00 - 09:30 Registration and Opening Session

09:30 - 10:00 Keynote Speaker: Maytal Caspary Toroker (Israel) CA18234 Chair
Toward multi-scale modeling of catalytic devices

Session 1 Quantum Mechanics

10:00 - 10:30 Keynote Speaker: Francesc Illas (Spain) WG1 leader
Electronic structure methods and models for water splitting with nanocrystals: where we are and where we go.

10:30 - 10:45 Invited QM talk 1: Jose Gomes (Portugal)
Water dissociation on two dimensional transition metal carbides or nitrides.

10:45 - 11:00 Invited QM talk 2: Dorota Rutkowska-Zbik (Poland)
Transition metal - based systems for applications in catalysis and photochemistry

11:00 - 11:30 COFFEE BREAK

11:30 - 11:45 Invited QM talk 3: Yuri Mastrikov (Latvia)
Multifaceted STO nanocrystals for water splitting

11:45 - 12:00 Invited QM talk 4: Konstantin Neyman (Spain)
Modelling nanocomposite materials for catalysis: From ceria to bimetallic crystallites

12:00 - 12:15 Invited QM talk 5: Bartłomiej Szyja (Poland)
Tuning the properties of hematite for its applications in photo-electrocatalysis

12:15 - 12:30 Invited QM talk 6: Stanislav Zalis (Czeck republic)
Modelling of photocatalytic water splitting at surface-modified nanomaterials

12:30 - 12:45 Invited QM talk 7: Ieva Barauskiene (Lithuania)
(Photo)electrocatalytic activity of cobalt based oxides in oxygen evolution reaction

12:45 - 13:00 Invited QM talk 8: Ángel Morales-García (Spain)
Structural and Electronic Properties of Realistic TiO_2 Nanoparticles

13:00 - 14:00 LUNCH BREAK

14:00 - 14:15 Invited QM talk 9: José C. Conesa (Spain)
Computing band alignments at semiconductor interfaces relevant to water splitting

14:15 - 14:30 Invited QM talk 10: Vicky Kozokaro (Israel)
LSFCr Perovskite as a Catalyst for CO_2 Reduction-Theoretical Insight into Reaction Mechanism

14:30 - 14:45 Invited QM talk 11: Roni Eppstein (Israel)
Electronic Structure of Oxide Spinels and Implications for Water Splitting

Session 2 Molecular Dynamics

14:45 - 15:15 Keynote Speaker: Nicolae Goga (Romania) WG2 leader
Molecular Dynamics Multiscaling

15:15 - 16:00 COFFEE BREAK

16:00 - 16:15 Invited MD talk 1: Leonard Mayerhofer (Germany)
Ab initio and classical MD investigations of solid-solid and solid-liquid interfaces.

16:15 - 16:30 Invited MD talk 2: Ionut Tranca (Netherlands)
DFT exploration of ORR and HER reactions on 2D materials

16:30 - 16:45 Invited MD talk 3: Koen Heijmans (Netherlands)
Molecular simulations for composite and doped thermochemical materials

16:45 - 17:00 Invited MD talk 4: Polina Tereshchuk (Israel)
Trends in the Adsorption of Oxygen and Li2O2 on Transition-metal Carbide Surfaces: A Theoretical Study

17:00 - 17:15 Invited MD talk 5: Ivan Rivalta (Italy)
Hybrid organic-inorganic nanoparticles: any hint from classical molecular dynamics simulations

17:15 - 17:30 Invited MD talk 6: Alessio Petrone (Italy)
Ab initio Molecular Dynamics towards time-resolved spectroscopies

Wednesday 12/02/2020

Session 3 Microscale and Continuum Modeling

09:30 - 10:00 Keynote Speaker: Anja Bieberle-Hütter (Netherlands) WG4 leader
Continuum Modeling for Electrochemical Applications

10:00 - 10:15 Invited MCM talk 1: Mehmet Arik (Turkey)
Recent Challenges in Microfluidics for Thermal Management of Micro/Nano Electronics

10:15 - 10:30 Invited MCM talk 2: Ivan RADOVIC (Serbia)
Theoretical modeling of experimental EELS data for supported and free-standing graphene

10:30 - 10:45 Invited MCM talk 3: Sergejs Pirkunovs (Latvia)
Multiscale modeling for water splitting application: Contribution from first principles.

10:45 - 11:00 Invited MCM talk 4: Greta Donati (Italy)
Joule effect at the nanoscale: a theoretical-computational model

11:00 - 11:30 COFFEE BREAK

11:30 - 13:00 WGs parallel meetings (5 rooms)

13:00 - 14:00 LUNCH BREAK

14:00 - 14:30 CG meeting (CA18234 Core Group members only)

14:30 - 16:00 *Assembly discussion + cooperation opportunities STSM ITC Conferences + website*

16:00 - 16:30 COFFEE BREAK

16:30 - 18:00 MANAGEMENT COMMITTEE MEETING

20:00 - 23:00 SOCIAL DINNER

Thursday 13/02/2020

Session 4 **Monte Carlo Simulations**

09:30 - 10:00 Keynote Speaker: Juan A. Anta (Spain) WG3 Vice leader
Monte Carlo Simulation of Electron Transport for Solar Energy Conversion: from Nanostructured Solar Cells to Water Splitting systems.

10:00 - 10:15 Invited MC talk 1: Vesselin Tonchev (Bulgaria)
Fractal dimension of ice on the nanoscale: A modelling approach (with verification of the analytical model)

Session 5 ***Multiscale Modeling***

10:15 - 10:30 Invited MM talk 1: Tomasz Adam Wesolowski (Switzerland)
Frozen-Density Embedding Theory approach to multi-level simulations of spectroscopic properties of molecules in condensed phase

10:30 - 10:45 Invited MM talk 2: Frederic Labat (France)
A generalized implicit solvation model for molecules, polymers, helices, nanotubes and surfaces

10:45 - 11:00 Invited MM talk 3: Anders Hellman (Sweden)
Challenges within the oxide-water interface

11:00 - 11:30 COFFEE BREAK

11:30 - 12:00 Keynote Speaker: Florian Libisch (Austria) WG5 leader
Multiscale description of catalysis: from embedding to large-scale models

12:00 - 12:15 Invited MM talk 4: Karoliina Honkala (Finland)
Kinetic modelling in catalysis

12:15 - 12:30 Invited MM talk 5: Aleix Comas-Vives (Spain)
Multiscale Modeling of Complex Heterogeneous Catalysts

12:30 - 12:45 Invited MM talk 6: Vesselin Tonchev (Bulgaria)
Self-regulating post-nucleation growth mode in two-dimensional nucleation (with validation).

13:00 - 14:00 LUNCH BREAK

14:00 - 15:00 ASSEMBLY DISCUSSION + CLOSING REMARKS

15:00 - 16:00 COFFEE BREAK