International Conference on Development of Nanocrystal Materials Through Computational Modelling // COST 18234 Meeting in ISRAEL

International Scientific Committee

- Maytal **Caspary Toroker** - Technion, Israel Institute of Technology, 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
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- José R. B. **Gomes** - University of Aveiro, Portugal
- Eugene **Kotomin** - University of Latvia, Latvia
- Tomasz **Wesolowski** - University of Geneva, Switzerland

Local Organizing Committee

- Maytal **Caspary Toroker** - Technion, Israel Institute of Technology, Israel
- Avi **Raveh**, Ministry of Science and Technology
- Smadar **Amir**, CA18234 Grant Manager

Scientific Program

Monday 17/07/2023

08:30 – 09:30	**Registration and Opening**	**Prof. Maytal Caspary Toroker, Chair of CA18234 and Prof. Michele Pavone, Vice Chair of CA18234**
	Session 1: Quantum Mechanics and Beyond Session Chair: José R. B. Gomes, University of Aveiro, Portugal	
09:30 - 10:00	Federico Calle-Vallejo	"Geometric effects on platinum electrocatalysts"
10:00 - 10:15	Anders Hellman	"Insights to the morphology of Fe2O3 clusters using computational methods"
10:15 - 10:30	Assa Sasikala Devi	"Tuning the properties of Janus van der Waals hetero structures by varying interface"
10:30 - 11:00	**Coffee Break**	
11:00 - 11:15	Bartłomiej Szyja	"Ru-pincer complexes as charge transfer mediators in CO2 reduction"
11:15 - 11:30	Piotr de Silva	"Singlet-triplet inversion in organic photoactive materials"
11:30 - 11:45	Veera Krasnenko	"Ab Initio Calculations of the Raman Spectra of Thin Strontium Titanate Films with and without Adsorbates"
11:45 - 12:00	Konstantin Neyman	"Effects of oxide supports on metal particles in catalytic nanomaterials"
12:00 - 12:15	Ugur Bozkaya	"Linear Scaling Coupled-Cluster Methods with Molecular Fragmentation Approaches"
12:15 - 12:30	Nadezda Kongi	"High-Performance Bifunctional Oxygen Electrocatalyst Derived from Bimetallic Mn/Co-MOF"
12:30 - 12:45	Klemen Bohinc	"Electrostatic and conductive properties of tubular structures"
12:45 - 13:00	Leonhard Mayrhofer	"Making green hydrogen even more sustainable – The substitution of PFAS in fuel cells and electrolyzers"
13:00 - 14:00	**Lunch Break**	
14:00 - 20:30	Visiting Tour + Social dinner	

Tuesday 18/07/2023

09:00 - 09:30	**Morning Coffee**	
Session 2: Atomistic to Microscale and Continuum Modeling Session Chair: Anders Hellman, Chalmers University of Technology, Sweden		
09:30 - 10:00	Michele Pavone	"Role of surface chemistry in tuning Oxygen red-ox catalysis at transition metal oxide surfaces"
10:00 - 10:30	Adriana Pecoraro	"Structural and electronic key features of Perovskite Solar Cells from First-principles"
10:30 - 11:30	**Coffee Break // Core Group meeting in parallel**	
11:30 - 12:00	Juan A. Anta	"First principles prediction of the low frequency behavior of perovskite materials and solar cells"
12:00 - 12:30	Guy Makov	"Novel nanometric phases of the monochalcogenides: Theory meets experiment"
12:30 - 13:00	Debesh R. Roy	"2D Metal Carbide Sensors for Environmentally Toxic Gasses under DFT and NEGF Approaches"
13:00 - 13:15	Tamar Goldzak	"Excited state phenomena and structural properties of nano-materials"
13:15 - 13:30	Nigel Clarke	"Organic Bulk Heterojunction Nanoparticles for Water Splitting"
13:30 - 15:00	**Lunch Break // Group Picture**	
15:00 - 16:00	MC MEETING (with Dr Emiljano KAZIAJ, SO COST Association)	
16:00 - 17:30	Poster Session	

Wednesday 19/07/23

08:30 - 09:00	**Morning Coffee**	

Session 3: Quantum Mechanics and Molecular Dynamics
Session Chair: Adriana Pecoraro, University of Naples Federico II, Italy

09:00 - 09:15	Mehmet Arik	"Early-stage frost formation and its effect on heat transfer: a fundamental approach to understand crystalline structure"
09:15 - 09:30	Luliana Marin	"Accelerating Molecular Dynamics Simulations with Enhanced GROMACS Algorithms and MPI Parallelization"
09:30 - 10:00	Jonny Bernstein	"First Principles Study of Rb Adsorption on Single-Layer Graphene/α-Al_2O_3 (0001) Interface"
10:00 - 10:15	Jose Gomes	"Insights into the structure and behavior of materials from classical MD simulations"
10:15 - 10:30	Stanislav Zalis	"Excited-state dynamics of photo-sensitizers containing heavy and earth abundant transition metals. Quantum mechanical and molecular dynamical study"
10:30 - 11:00	Nicolae Goga	"Developments in Multiscaling Simulations"
11:00 - 11:30	**Coffee Break**	

Session 4: Single-scale, Multiscale Modeling and Machine learning
Session Chair: Nicolae Goga, Polytechnic of Bucharest, Romania

11:30 - 12:00	Tomasz Wesolowski	"Frozen-Density Embedding Theory based multi-scale simulations of the effect of environment on the electronic structure of solvated species"
12:00 - 12:30	Florian Libisch	"Multi-scale simulation of large-scale nanostructures: combining tight-binding and DFT"
12:30 - 12:45	Said Hamad Gomes	"Study of the nucleation of ZIFs via machine learning potentials"
12:45 - 13:00	Ricardo Grau-Crespo	"Designing nano-structured chalcogenides for thermoelectric applications using density functional theory and machine learning"
13:00 - 14:00	**Lunch Break**	

Session 5: From First Principles to Monte Carlo Simulations

Session Chair: Florian Libisch, Vienna University of Technology, Austria

14:00 - 14:30	Arik Yochelis	"Micro-Kinetic Approach to Photo-Electrochemical Water Splitting: Uncovering Novel Reaction Pathways"
14:30 - 15:00	Amir Natan	"Oxygen Reduction Reactions at metal and other surfaces"
15:00 - 15:15	Titus van Erp	"Pushing the Limits of Time Scales in Molecular Simulation"
15:15 - 15:30	Vesselin Tonchev	"Quantifying the growth order in "artificial" crystallization"
15:30 - 15:45	Peter Vansco	"Unique electronic properties of rhombohedral graphite thin films"
15:45 - 16:00	Dimitry Bocharov	"Titanium Dioxide: Bridging Photocatalytic Processes and Antibacterial Activity"
16:00 - 16:30	**Assembly Discussion + Closing Remarks**	
16:30	**Farewell Coffee**	

Poster Session 18/07/2023

1. **Andreas Douloumis:** Electronic structure of photocatalytic materials: doped ZnO and gold-perovskite interfaces
2. **Andreu de Donato:** Global optimization and thermodynamic phase diagrams of IrOx particles
3. **Dorota Rutkowska-Zbik:** DFT studies on Cu_n/TiO2 (n=1-6) system for water splitting
4. **Ivan Radovic:** Wake potential in graphene-insulator-graphene heterostructure: the role of graphene-insulator distance
5. **Labanya Bhattacharya:** Nature of Potential Energies at Different Levels of Theory for Different Perovskite Solar Cell Building Blocks
6. **Lakhanlal Lakhanlal:** Study of heat treated γ-NiFeOOH aerogel for oxygen evolution reaction using DFT
7. **Neeraj Mishra:** Nanoscale growth of metastable π-SnS by impurity addition or choice of substrate
8. **Noam Hadari:** An Efficient Model to Describe Lattice Mismatched Interface System
9. **Radhey Yadav:** Tri-metallic alloys as an electro-catalyst for fuel cells – The case of MF on Pt3Pd3Sn2
10. **Ricardo Urrego-Ortiz:** How DFT Errors Spread in Computational Electrocatalysis Models
11. **Shkëndije Haziri Sefa:** Using MC Simulation to study the solution/solvent interaction between O_2 formed on the surface of hematite.
12. **Veton Haziri:** Theoretical and EIS investigation of the formation of oxygen on the surfaces of different materials.
13. **Kumar Vipin:** Oxygen reduction reaction on pristine and N-doped nanosheet comparison study by implicit and explicit solvent model