CA18234. COMPUTATIONAL MATERIALS SCIENCES
FOR EFFICIENT WATER SPLITTING WITH NANOCRYSTALS
FROM ABUNDANT ELEMENTS

MOLECULAR DYNAMICS FOR TREATING NANOSCALE MATERIALS

TUESDAY // 01 DEC. 2020 // PROGRAM

10:00-10:30 OPENING

MAYTAL CASPARY TOROKER ▸
The future of modeling nanoscale catalysts

NICOLAE GOGA ▸
Molecular Dynamics and its value

10:30-12:30 SESSION 1

MARTIN PRESSELT ▸ Developing and modelling organic membranes for photo-energy conversion, Leibniz-Institute of Photonic Technologies, Germany

MAYRHOFER ▸ Leonhard, Facile and Efficient Atomic Hydrogenation Enabled Black TiO2 with Enhanced Photo-Electrochemical Activity via a Favorably Low-Energy-Barrier Pathway, Fraunhofer Institute, Germany

KOEN HEIJMAN ▸ Development of a reactive water force field for molecular simulations, Eindhoven University of Technology, the Netherlands

POPA RAMONA & GOGA NICOLAE ▸ Artificial intelligence algorithms used in molecular dynamics, Politehnica University of Bucharest, Romania

12:30-13:30 BREAK

13:30-16:30 SESSION 2

MIKAEL VALTER ▸ Solvent Effects for Methanol Electrooxidation on Gold, Chalmers University, Sweden

D. BOCHAROV ▸ Ab initio molecular dynamics simulations for EXAFS interpretation and developement of empirical potentials, University of Latvia, Riga

S. PISKUNOV ▸ Modelling of nanotubes for visible-light-driven, photocatalytic water splitting and development of 2D periodic model approximations for molecular dynamics simulations, University of Latvia, Riga

MOVAFFAQ KATEB KATESHAMSHIR ▸ Point defect dynamic at the catalyst surface, Reykjavik University, Iceland

KLEMEN BOHINC ▸ Charge properties of TiO2 nanotubular structures, University of Ljubljana, Slovenia

CARLO ADAMO ▸ Non-empirical density functionals: where we are, what we can and what we cannot do, Institut Universitaire de France, France

NOTES
1. All presentations are virtual
2. Each presentation holds 25 minutes with 5 minutes questions