

**List of MD Group Conference Presentations in Bulgaria,
August 23 and 24, 2021**

Day 1, Monday August 23, 2021

Session 1, 11-11.30 – Opening (face-to-face and virtual)

- Maytal Toroker, Chair Cost Action 18234
- Nicolae Goga, Chair Molecular Dynamics Group

Session 2 – Presentations face-to-face and online, 11.30-12.30

- Eitan Yohanan, *The effect of interlayer stacking arrangements in two dimensional NiOOH on water oxidation catalysis*, Technion University, Israel.
- Dinu Bianca, *DPD Thermostat For Water Splitting*, Polytechnic University of Bucharest, Romania

Break 1, 12.30-14

Session 3 – Presentations face-to-face and online, 14 -15

- Boros Mihai, *Implementation of DPD Thermostat*, Polytechnic University of Bucharest, Romania
- Viktor Zhukovskyy, *Mathematical and Computer Modelling of Contaminant Migration in Porous Media with Nanoparticles*,

Break 2, 15-15.15

Session 4 – Molecular Dynamics Group discussions 15.15 – 17

Day 2, Monday August 24, 2021

Session 1 – Presentations face-to-face and online, 11-12.30

- Veerapandian Ponnuchamy, *Towards understanding of the photochemical water splitting process: A molecular dynamics perspective*, InnoRenew, Slovenia
- Bartek Szyja, *Stability of TiO₂ clusters supported on Fe₂O₃*, Wroclaw University of Science and Technology, Poland
- Klemen Bohinc, *Morphological and Charging Properties of Nanoparticles*, University of Ljubljana, Slovenia

Break 1, 12.30-14

Session 2 – Presentations face-to-face and online, 14 -15

- Alexandru Bratosin, *Artificial Intelligent algorithms in Molecular Dynamics*, Polytechnic University of Bucharest, Romania
- Cristian Taslitchi, *Developments in multiscaling simulations*, Polytechnic University of Bucharest, Romania

Break 2, 15-15.15

Session 4 – Molecular Dynamics Group discussions 15.15 – 17