

**List of MD Group Conference Presentations in Crete,  
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

- Georgios Kopidakis, *Theoretical investigation of transition metal dichalcogenide nanostructures for hydrogen evolution*, University of Crete, Greece
- Veerapandian Ponnuchamy, *Towards understanding of the photochemical water splitting process: A molecular dynamics perspective*, InnoRenew, Slovenia

Break 1, 12.30-14

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

- Dinu Bianca, *DPD Thermostat For Water Splitting*, Polytechnic University of Bucharest, Romania
- Boros Mihai, *Implementation of DPD Thermostat*, Polytechnic University of Bucharest, Romania

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**

- Eitan, *The correlation between interlayer arrangements in two dimensional NiOOH and its catalytic performance on water splitting*, Technion University, Israel.
- Bartek Szyja, *Stability of TiO<sub>2</sub> clusters supported on Fe<sub>2</sub>O<sub>3</sub>*, 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, *Computational Algorithms for material science*, Polytechnic University of Bucharest, Romania

### **Break 2, 15-15.15**

### **Session 4 – Molecular Dynamics Group discussions 15.15 – 17**