



Faculty of Chemistry and Pharmacy
University of Sofia



COMPUTATIONAL MODELING OF MATERIALS SCHOOL

04-05 DECEMBER 2017

*CONFERENCE HALL
FACULTY OF CHEMISTRY AND PHARMACY
UNIVERSITY OF SOFIA*

Program

Monday, 4th December

10:00	Opening – Georgi Vayssilov
10:10	Pablo Gamallo – University of Barcelona, Spain “Molecular Dynamics Simulations Applied to Industrial Processes”
11:00	<i>Coffee break</i>
11:20	Stefan Bromley – University of Barcelona, Spain “Exploring the Potential Energy Landscape of Inorganic Materials: from Nanoscale to Bulk”
12:10	<i>Break</i>
14:00	Eliseo Ruiz – University of Barcelona, Spain “Efficient Transport and Magnetoresistance Effect in Single-Molecule Devices”
14:50	<i>Coffee break</i>
15:10	Sergio Madurga – University of Barcelona, Spain “Simulation Techniques for Soft Materials”
16:00	<i>Coffee break</i>
16:20	Stefan Bromley – University of Barcelona, Spain “How to give Successful Scientific Presentations”
17:10	<i>Enjoy your evening</i>

Tuesday, 05th December

09:30	Ivelina Georgieva – Bulgarian Academy of Sciences, Bulgaria "Molecular Modeling of Optical Properties of Lanthanide Complexes and Chromophores"
10:20	<i>Coffee break</i>
10:30	Yuki Nagata - Max-Planck Institute for Polymer Research, Germany "Molecular Modeling of Ice and Water Surfaces; Input from the Oretical Sum-frequency Generation Spectroscopy"
11:20	<i>Coffee Break</i>
11:30	Jorge Echeverría – University of Barcelona, Spain "Noncovalent Interactions: A useful Tool for Crystal and Materials Design"
12:20	<i>Break</i>
14:00	Jordi Cirera – University of Barcelona, Spain "Modelling Spin-crossover in Condensed Phase: From Molecules to Metal-Organic Frameworks"
14:50	<i>Coffee break</i>
15:00	Presenting the groups from the Faculty of Chemistry and Pharmacy that work on Computational Chemistry
16:00	<i>Coffee break</i>
16:20	Ivan Vakarelski - King Abdullah University of Science and Technology, Saudi Arabia "Objects with Near-zero Hydrodynamic Resistance"
17:10	<i>Enjoy your evening</i>
