



COMPUTATIONAL MODELING OF MATERIALS SCHOOL

04-05 DECEMBER 2017

FACULTY OF CHEMISTRY AND PHARMACY

UNIVERSITY OF SOFIA

SOFIA, BULGARIA

Program

Conference Hall of the Faculty of Chemistry and Pharmacy, Sofia University

Monday, 4th December

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| 10:00 | Opening – Georgi Vayssilov |
| 10:10 | Pablo Gamallo – University of Barcelona, Spain “Molecular dynamics simulations applied to industrial processes” |
| 11:00 | Coffee break |
| 11:20 | Stefan Bromley – University of Barcelona, Spain “Exploring the Potential Energy Landscape of Inorganic Materials: from Nanoscale to Bulk” |
| 12:10 | Break |
| 14:00 | Eliseo Ruiz – University of Barcelona, Spain “Efficient Transport and Magnetoresistance Effect in Single-Molecule Devices” |
| 14:50 | Coffee break |
| 15:10 | Sergio Madurga – University of Barcelona, Spain “Simulation Techniques for Soft Materials” |
| 16:00 | Coffee break |
| 16:20 | Ivelina Georgieva – Bulgarian Academy of Sciences, Bulgaria "Molecular modeling of optical properties of lanthanide complexes and chromophores" |
| 17:10 | Enjoy your evening |

Tuesday, 05th December

09:30 Stefan Bromley – University of Barcelona, Spain
“How to give Successful Scientific Presentations”

10:20 *Coffee break*

10:30 Yuki Nagata - Max-Planck Institute for Polymer Research, Germany
“Molecular modeling of Ice and water surfaces; Input from theoretical sum-frequency generation spectroscopy”

11:20 *Coffee Break*

11:30 Jorge Echeverría – University of Barcelona, Spain
“Noncovalent interactions: A useful tool for crystal and materials design”

12:20 *Break*

14:00 Jordi Cirera – University of Barcelona, Spain
“Modelling Spin-crossover in condensed phase: From molecules to Metal-Organic Frameworks”

14:50 *Coffee break*

15:00 Presenting the groups from the Faculty of Chemistry and Pharmacy that work on Computational Chemistry

16:00 *Coffee break*

16:20 Ivan Vakarelski - King Abdullah University of Science and Technology,
Saudi Arabia
"Objects with near-zero hydrodynamic resistance"

17:10 *Enjoy your evening*
