Program for The 4th EMN Meeting on Computation and Theory *Sept 3 – 7, San Sebastian, Spain*		
Monday, Sept 3 **Registration** **Time: 14:00~17:00**		
Tuesday morning, Sept 4 **Room A**		
Opening: 8:55-9:00		
Session: DFT I Chair: Jianmin Tao		
9:00-9:25	A01: Linear response in topological semimetals	**Yan Sun** Max Planck Institute for Chemical Physics of Solids, Germany
9:25-9:50	A02: Optical spectra from first principles: fundamentals, functionals, and numerics	**Arjan Berger** Université Paul Sabatier, France
9:50-10:15	A03: Structural modelling for (Ag2Te)x(AsTe)1-x glasses by a combination of reverse Monte Carlo modelling and density functional theory	**Shuta Tahara** University of the Ryukyus, Japan
10:15-10:30	Coffee Break	
Session: General I Chair: Mark Eberhart		
10:30-10:55	A04: On the inclusion of dissipative effects in clusters and molecule	**Eric Suraud** LPT Toulouse - Université Paul Sabatier, France
10:55-11:20	A05: Four-component coupled cluster study of small actinide species: ground and excited state properties	**Paweł Tecmer** Nicolaus Copernicus University in Toruń, Poland
11:20-11:45	A06: Molecules in Strong Magnetic Fields	**Sangita Sen** University of Oslo, Norway
11:45-12:10	A07: A simplified solution of Coupled Cluster equations by utilization of scaled MP2 amplitudes.	**Szymon Śmiga** Nicolaus Copernicus University, Poland

Tuesday afternoon, Sept 4 Room A		
Session: DFT II Chair: Yan Sun		
14:00-14:25	A08: Kinetic Energy Functionals for Orbital-Free Density Functional Theory	**Lucian Constantin** Istituto Italiano di Tecnologia(ITT), Italy
14:25 -14:50	A09: TBD	**Jianmin Tao** Temple University, USA
14:50 -15:15	A10: Density functional electric response properties of atoms and molecules in Cartesian grid	**Amlan Kusum Roy** Indian Institute of Science Education and Research (IISER)-Kolkata Mohanpur Campus, India
15:15-15:40	A11: Manipulation of the two- and four-photon Hong-Ou-Mandel interference	**Polina Sharapova** University Paderborn, Germany
15:40-15:55	Coffee Break	
Session: General II Chair: Eric Suraud		
15:55-16:20	A12: Is there a preferred charge density reference frame?	**Mark Eberhart** Colorado School of Mines, USA
16:20-16:45	A13: Atomic / Ionic Radius as Mathematical Limit of System Energy Evolution	**Paweł Szarek** University of Warsaw, Poland
16:45-17:10	A14: A stochastic equation for tensile fracture of polymeric solids	**Koh-hei Nitta** Kanazawa University, Japan
17:10	Dinner Social	

Wednesday morning, Sept 5 Room A		
Session: DFT III Chair: Robert Gyepes		
9:00-9:25	A15: Pincer Metal Catalysts for Green Chemistry	**Albert Poater** IQCC, University of Girona, Spain
9:25-9:50	A16: Effect of van der Waals interaction on band mobility of organic semiconductors	**Hajime Kobayashi** Advanced Technology Research Division, Sony Corporation, Japan
9:50-10:15	A17: Gradient-dependent exchange-correlation kernel for materials optical properties	**Aleksandr Terentjev** Donostia International Physics Center (DIPC), Spain
10:15-10:30	Coffee Break	
Session: Molecular Electronics Chair: Albert Poater		
10:30-10:55	A18: Computational Studies of Unusual Bonding Modes in Complexes with Transition Metals	**Robert Gyepes** Charles University, Czech Republic
10:55-11:20	A19: From tight-binding Hamiltonians to low-temperature thermoelectric properties of bilayer graphene	**Adam Rycerz** Jagiellonian University, Poland
11:20-11:45	A20: Charge Transport in Lamellar Structure of Linear Conjugated Polymers	**Petr Toman** Ústav makromolekulární chemie AV ČR, v.v.i. (ÚMCH), Czech Republic
11:45-12:10	A21: Modeling ground and excited states with germinal-based approaches	**Katharina (Kasia) Boguslawski** Nicolaus Copernicus University, Poland

Wednesday afternoon, Sept 5 Room A		
Session: Molecular Dynamics and its Applications		**Chair: Lucian Constantin**
14:00-14:25	A22: Critical Vaporization of MgSiO3: A First Principles Molecular Dynamics Simulations	**Bing Xiao** Xi'an Jiaotong University, China
14:25 -14:50	A23: Large-Scale DFT Molecular-Dynamics Simulation of Organic Molecules@SWCNT for Li-ion Battery Electrode	**Shuji Ogata** Nagoya Institute of Technology, Japan
14:50 -15:15	A24: Hybrid Quantum-Classical Dynamics Simulation of Moisture-Induced Weakening of Metal-Resin Adhesion	**Shuji Ogata** Nagoya Institute of Technology, Japan
15:15-15:40	A25: Effect of alkyl branches on the thermal stability of quaternary ammonium cations	**Yong Nam Ahn** Corning Technology Center Korea, Korea
15:40-16:05	A26: New Dichalcogenides as Crosslinks for Efficient Self-Healing Materials	**Fernando Ruiperez** POLYMAT, University of the Basque Country UPV/EHU, Spain
16:05-17:00	**Poster** (&Coffee Break)	
P01: DFT modeling of Redox Potentials of full Organic Dyes for Dye-Sensitized Solar Cells		**Sanaz Mohammadpourasl** University of Florence, Italy
P02: A meta-GGA level screened range-separated hybrid functional by employing short range Hartree–Fock with a long range semilocal functional		**Subrata Jana** National Institute of Science Education and Research, India
P03: Diastereoisomerism in platinum(II) phosphino- and aminothiolato hydrido complexes		**Alfons Polo** University of Girona, Spain
P04: Characterization of air-saturated porous materials using ultrasonic reflected waves - frequency approach		**Mustapha Sadouki** Université Djilali Bounaama de Khemis-Miliana, Algeria
17:00PM	Dinner Social	

Thursday morning, Sept 6 Room A		
Session: DFT IV Chair: Nina P. Gritsan		
9:00-9:25	A27: Defect Formation Energies Due to Hydrogen-dopants on Interstitial Sites in Uranium Intermetallic Compounds	**Bun Tsuchiya** Meijo University, Japan
9:25-9:50	A28: Mechanisms of Metallocene Catalysts Activation in Ziegler-Natta Type Processes	**Tatyana V. Tyumkina** Institute of Petrochemistry & Catalysis, RAS, Russia
9:50-10:15	A29: Theoretical challenges and issues for the design of high energy density material for Li-ion batteries	**Matthieu Saubanère** Institut Charles Gerhardt Montpellier, France
10:15-10:30	Coffee Break	
Session: General III Chair: Matthieu Saubanère		
10:30-10:55	A30: Combination Law for Electron Damping in Multilayer Thin Metal Films	**Stefano A. Mezzasalma** Institut Ruđer Bošković, Croatia
10:55-11:20	A31: On the optimal basis set for electron dynamics in strong laser fields : the case of H+2	**Eleonora Luppi** Université Pierre et Marie Curie - CNRS, France
11:20-11:45	A32: Theoretical Study on the Charge Transfer Mechanism at Donor/Acceptor Interfaces	**Koichi Yamashita** The University of Tokyo, Japan
11:45-12:10	A33: TBD	**Subhasish Mandal** Yale University, USA

Thursday afternoon, Sept 6 Room A		
Session: DFT V & Materials Predictions		**Chair: Eduardo Fabiano**
14:00-14:25	A34: Electronic structure, spectroscopy and magnetic properties of niroxide radicals, diradical and their complexes with transition metals: ab initio and DFT study	**Nina P. Gritsan** Novosibirsk State University, Russia
14:25 -14:50	A35: Boron, the most multi-structure material ever: a first principles study	**Nevill Gonzalez Szwacki** University of Warsaw, Poland
14:50 -15:15	A36: Materials Characteristics Prediction: Case of Stainless Steels	**Goran Vukelić** University of Rijeka, Croatia
15:15-15:40	A37: First-principles approach of the properties of materials for production and storage of energy	**Philippe Baranek** EDF R&D, Ile – de – France Photovoltaic Institut (IPVF), France
15:40-15:55	Coffee Break	
Session: DFT VI		**Chair: Eric Suraud**
15:55-16:20	A38: Approximate functionals based the adiabatic connection applied to main group, non-covalent, and metals chemistry	**Eduardo Fabiano** Istituto Italiano di Tecnologia, Italy
16:20-16:45	A39: Modelling of adsorption and intercalation of hydrogen on/into tungsten disulphide multilayers and multiwall nanotubes	**Jose Ignacio Martinez Ruiz** Instituto de Ciencia de Materiales de Madrid, CSIC, Spain
16:45-17:10	A40: Orbital-dependent improvements to density-functional approximations: Applications of the FLO-SIC method	**Torsten Hahn** Technische Universität Bergakademie Freiberg, Germany
17:10-17:35	A41: The Linear Response Function in Conceptual DFT : recent Insights and Applications	**Paul Geerlings** Vrije Universiteit Brussel - VUB, Belgium
17:35	Dinner Social	