THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELING: 20 YEARS PROMOTING EXCELLENCE IN SCIENCE (20TCCM)

THURSDAY (30 May)			FRIDAY (31 May)	SATURDAY (1 June)
		9:00-9:50	Alicia Palacios "Exploring ultrafast molecular dynamics using attosecond pulses: from H2 to amino acids."	Ferran Frixas "Accelerating (Bio)molecular Recognition and Assembly with Molecular Dynamics Simulations"
		9:50-10:10	Javier Cerezo "Unraveling the energetic contributions in protein folding"	Oriana Brea Modeling the Thermal Decomposition of N-nitrosoamides
		10:10-10:30	Elixabete Rezabal "Development Of New Photoactivatable Anticancer Prodrugs"	
		10:30-10:50	Jon Mattin Matxain "Computational-Experimental Development of Self Healing Polymers with Dichalcogenide Cross-Links "	Daniel J. Arismendi-Arrieta CONFINING SOFT NANOPARTICLES AT LIQUID-LIQUID INTERFACES
		10:50-11:10	Rodrigo Casanovas Computational Approaches to understanding Protein Glycation and its Biological ImplicationsOral Contribution	Cristina Roncero Magnetic and Conductive properties in multifunctional bisdithiazolyl based materials
		11:10-11:30	**COFFEE BREAK**	**COFEE BREAK**
		11:30-12:00	Sergio Martí The QMCube framework	Jose Javier Ruiz-Pernia The role of thermal stability in enzyme catalysis.
		12:00-12:20	Jose Javier Plata "Photo-sensitizing ferroelectric oxides using materials databases and highthroughput calculations	Anna S. Bondarenko Computational Modeling of Structure and Excitonic Properties of Molecular Nanotubes
		12:20-12:40	Olatz Uranga-Barandiaran Photophysics of Molecular Aggregates from Excited State Diabatization	Selim Sami Computation of the dielectric constant and its importance for organic photovoltaics
		12:40-13:00	Cesar Menendez Magneto-structural phase transitions in multiferroic $BiCoO_3$ thin films	**Concluding Remarks** Manolo Yañez 12:40:13:10
		13:00-15:00	**LUNCH**	
16:00-16:45	**REGISTRATION**	15:00-15:50	Daniel Roca-Sanjuán Chemistry of the excited electronic state induced by UV-Vis photons and chemical energy	**2:30 Lunch @Gastronomica**
16:45-17:00	**Oppening** Jesus M. Ugalde	15:50-16:20	Maria Basora Bond Dissociation Energies, what are made out of?	
17:00-17:50	Julia Contreras-Garcia ***From errors in the density to calculated error bars***	16:20-16:40	Javier Carrasco ***"On the Atomistic Modelling of Battery Materials"***	
17:50-18:20	Lola Gonzalez MgH- and MgH+: ionic state-changing collisions in cold traps	16:40-17:00	Joaquim Jornet-Somoza Transition Density Formulation from TDDFT Enables Exciton Coupling Calculations in Large Systems	
18:20-18:50	Eduard Matito Salient signature of van der Waals interactions	17:00-19:00	**Coffee Break & Poster Session**	
19:00-20:30	**WELLCOME COCKTAIL**			