METHODLODOGY			
General keyword	**Details in topic**	**Researchers involved**	**Insitiute (Group Acronym)**
Development of electronic structure methods	Development of new density functional aproximations	Eloy Ramos, Rubén Ferradás, Eduard Matito	UPV/EHU-DIPC (QCDG)
	Study of Electron Correlation	Eloy Ramos, Rubén Ferradás, Eduard Matito	
	Density Matrix Functional Theory	Eloy Ramos, Eduard Matito	
Aromaticity	Development of tools to analyze aromaticity	Eloy Ramos, Eduard Matito	

Methodology for Molecular Dynamics Simuations	Atomistic molecular dynamics of biomolecules	David De Sancho, Xabier López
	Force field development and refinement	David De Sancho, Xabier López
	Coarse-grained modelling of protein-protein interactions	David De Sancho
	Network models for molecular kinetics, Markov state models	David De Sancho
Electronic structure methods	Development and implementation of electronic structure methods for computation and characterization of ground and excited states	

Quantum master equations	Development and implementation of quantum master equation methods for exciton dynamics	David Casanova		
Kinetic Monte Carlo	Development and implementation of kinetic Monte Carlo program for energy/charge transport			
APPLICATIONS				
Systems	**Property**	**Methods**	**Researchers involved**	**Insitiute (Group Acronym)**
Aromaticity	Study of new aromatic molecules. All-metal clusters.	QTAIM, Electron delocalization, Magnetizabilities	Eduard Matito, J. M. Mercero	UPV/EHU-DIPC (QCDG)

Gold NP - PTEBS interface	Photochemistry, Interface Structure, electron transfer	DFT, TDDFT, Molecular Dynamics, Quantum Molecular Dynamics	Jon M. Matxain	UPV/EHU-DIPC (KT-JMM)
Polymer - Metal Oxides	Interaction energies, Mechanical Properties, Photochemical properties, Self-Healing		Jon M. Matxain	
Surface supported precious metals nanoclusters for their use as catalysts	Catalytic properties, cataytic selectivity, tendency to poison or deactivate	Plane waves DFT, Perriodic Boundary Conditions, Chemical bonding analysis tools	Elisa Jimenez-Izal, Jose M. Mercero	UPV/EHU-DIPC (KT-EJI)
Deep eutectic solvents for biomass treatment	Lignin solvation and depolimerization mechanism by deep eutectic solvents		Elixabete Rezabal, Jon Zubeltzu	

Photoactivation of anticancer metallic prodrugs by flavines	NOX and miniSOG protein dynamics, organometallic complex docking, flavine redox and optical properties, prodrug activation mechanism	Classical MD, ab initio MD, DFT, TDDFT, aNCI	Elixabete Rezabal, Xabier Lopez, Luca Salassa	UPV/EHU-DIPC (KT-ERA)
Intrinsically disordered proteins	Biophysics / Dynamics / Interactions	Atomistic MD simulations / Coarse graining / Force fields	David De Sancho, Xabier López	UPV/EHU-DIPC (BioKT)
Amyloids				
Phase behaviour of protein mixtures				
Protein-metal interactions	Protein-metal interactions	Atomistic MD simulations / DFT / Force fields / Analysis tools		

organic molecules / molecular aggregates / molecular solids	Electronis states and interactions: charge transfer, exciton delocalization, spin-orbit, spin-spin and hyperfine interactions.	Electronic structure methods: WFT, DFT, WFT-DFT / TDDFT / spin-flip / Model and Effective Hamiltonians	David Casanova	UPV/EHU-DIPC (KT-DCC)
	Photophysics and photochemistry: delayed emission, ISC, singlet fission, triplet-triplet annihilation	Quantum master equations		
	Exciton transport / charge transport / charge recombination	kinetic Monte Carlo		