METHODOLODOGY		
General keyword	**Details in topic**	**Researchers involved**
Solvent representation in Monte Carlo simulations using QM/MM Multiconficuracional methodology for excited states	QM/MM hybrid Hamiltonians	Jose M. Hermida
	Description of the intermolecular terms between the QM and Clasical systems	Jose M. Hermida
	Improvement of the computational cost of the polarization term	Jose M. Hermida
Electron transport in molecular devices	Study of the electric conductance in molecular wires and molecular rectifiers using electron deformation orbitals, a new methodology of general application for HF, post-HF and DFT levels developed and implemented in the quantum chemistry group of the University of Vigo	Marcos Mandado Alonso

Energy decomposition analysis (EDA)	Energy decomposition analysis of non-covalent intermolecular interactions based on electron deformation densities. Developments for QM and QM/MM hamiltonians and for two and more than two interacting systems.	Marcos Mandado Alonso	
APPLICATIONS			
Systems	**Property**	**Methods**	**Researchers involved**
Gold catalysis	Reaction mechanism, kinetics, selectivity, nature of the gold-substrate bond	DFT, post-HF when necessary	Olalla Nieto Faza / Carlos Silva Lopez
Valorization of biomass processing by-products	Oxygen atom abstraction processes, polyoxovanadate and polyoxomolibdate catalysis, reaction mechanisms, surface crossing events	DFT, port-HF, Multiconfigurational SCF	Olalla Nieto Faza / Carlos Silva Lopez
Bispericyclic reactions	Reaction dynamics, quasi-classical trajectories, path bifurcations, valley-ridge inflection points	DFT, BOMD, AIMD	Olalla Nieto Faza / Carlos Silva Lopez
Small molecular systems of astrophysical relevance.	Structural and dynamical properties	High accuracy electronic structure methods (MRCI, CC, F12 methods, spin-orbit and relativistic methods, Vibrational CI methods, etc.). (b) TST and RRKM theories. Instanton Methods. QCT methods. SC-TDSE based methods (i.e. Tully's FSTSH)	Jesús Flores
Small molecular systems of astrophysical relevance.			
Metal Clusters	Structural, electric, magnetic properties. Reactivity and dynamical properties	DFT, Relativistic DFT methods, RPA-based methods, GW, BSE methods.	Jesús Flores

Reactions between a solvated electron and nucleotides in ground and excited state	Reaction mechanism. States involved. Charge tranference. Solvation energy	CASSCF, CASPT2, RASSCF, RASPT2, DMRG	Jose M. Hermida
Molecular Tweezers complexes with ionic species	Binding energy. Energy Barriers. Electronic densities	EDA. SAPT. DFT. TDDFT. AIMD. MD-QM/MM	Marcos Mandado/Jose M. Hermida
Solvation of ionic species	Solvation energy.	EDA. SAPT. DFT. TDDFT. AIMD. MD-QM/MM	Jose M. Hermida
Spectrum and Excited States of Large Molecules	wavelenght, intensities. NTO. Orbitals, Densities.	CASSCF, CASPT2, RASSCF, RASPT2, DMRG	Jose M. Hermida
Adsorption of molecules on graphene and related surfaces	Interaction energy. Free energy	DFT, EDA, Quantum Chemical Topology (QCT)	Marcos Mandado Alonso
Optical properties of hybrid boron, nitrogen, carbon materials (h-BNCs)	Polarizability, hiperpolarizabilities, transition density, difference density	DFT, TDDFT, CPDFT	Nicolas Oero Martínez/Marcos Mandado Alonso