Universidad de Oviedo

METHODOLODOGY			
General keyword	Details in topic	Researchers involved	Insitiute (Group Acronym)
Extending the Interacting Quantum Atom approach towards biomolecular systems	Fragment-based assessment of numerical errors in IQA calculations.	Dimas Suárez, Natalia Díaz	UniOvi (QTCOVI)
	Inclusion of solvent & environmental effects into QM and QM/MM IQA calculations	Dimas Suárez, Natalia Díaz	
	Improvement of the computational tools required for DFT-D3 IQA calcualtions on large systems.	Dimas Suárez, Natalia Díaz	

Computational Chemistry of Materials	Development of affordable computational methods for structural prediction of organic electronic matrials	Alberto Otero		
Computational Chemistry of Materials	Delocalization and strong correlation errors in DFT by means of correcting atom-centered potentials	Alberto Otero		
Advances in Quantum Chemical Topology	Quantum atoms as open quantum systems	Ángel Martín Pendás, Evelio Francisco, Aurora Costales	Javier Junquera	
Advances in Quantum Chemical Topology	Chemical bonding in excited states	Ángel Martín Pendás, Evelio Francisco, Aurora Costales	Pablo García-Fernández	
Advances in Quantum Chemical Topology	Atoms in molecules and maxima of the square of the wavefunction	Ángel Martín Pendás, Evelio Francisco, Aurora Costales	José Antonio Aramburu and Pablo García-Fernández	

APPLICATIONS				
Systems	**Property**	**Methods**	**Researchers involved**	**Insitiute (Group Acronym)**
DNA aptamers and peptide targets	Secondary and tertiary structures of aptamers. Aptamer-protein binding determinants.	Gaussian-Accelerated and conventional MD, AutoDock, End-point free energy methods (MM-PBSA)	Natalia Díaz, Dimas Suárez	UniOvi (QTCOVI)

Rhenium and Molybdenum Carbonyl Diimine Complexes with organic or inorganic monodentate ligands	Spectroscopy, Magnetism Aromaticity, Photophysics, Photocytotoxicity, Solvation	DFT, TD-DFT, PCM, CPCM, NICS, Magnetically Induced Current Density (MICD)	M. Isabel Menéndez Ramón López Daniel Álvarez	UniOvi (QTCOVI)
Metal Complexes of Groups VI, VII, and VIII against organic and biological substrates	Geometry, Thermochemistry, Kinetics, Atomic Charge, Dipole Moment, Electrostatic Molecular Potential, Solvation	WFT, DFT, NBO, AIM, PCM, CPCM	M. Isabel Menéndez Ramón López Daniel Álvarez	UniOvi (TEQO)
Porphyrin derivatives-BODIPY adducts	Geometry, Spectroscopy, Aromaticiy, Magnetism, Photophysics, Photocytotoxicity	DFT, TD-DFT, NICS, MICD	M. Isabel Menéndez Ramón López Daniel Álvarez	Uniovi (TEQO)
Chiral Crytals			J. M. Recio	Uniovi (QTCMAT)

Composition of Exoplanets			J. M. Recio	Uniovi (QTCMAT)
Thermoelectric Materials			J. M. Recio	Uniovi (QTCMAT)
Electron delocalization in materials under pressure			Alberto Otero	Uniovi (QTCMAT)
IQA in chemical reactions	Energy decomposition	WFT, CAS, CI, DFT	Ángel Martín Pendás, Evelio Francisco, Aurora Costales	UniOvi (QTCOVI)
Electron distribution function analysis	Electron occupation, Lewis structures	WFT, CAS, CI, DFT	Ángel Martín Pendás, Evelio Francisco, Aurora Costales	UniOvi (QTCOVI)
Effect of non-covalent interactions in mlecular crystals structure	Non-covalent interactions, crystal structures, Atomic charge	DFT, ELF, NCI, AIM, Global optimization	Julen Munárriz	UniOvi (QTCOVI)
Modelling realistic cluster-decorated electro-catalytic interfaces	Geometry, electrocatalysis, ORR, OER, external potential, solvation	DFT, Poisson-Boltzmann equation, Global optimization, implicit solvation models,	Julen Munárriz	UniOvi (QTCOVI)

Development of Co/Rh/Ir-based catalysts for the dehydrogenation of formic acid. Use of formic acid as a "green" energy vector	Geometry, Thermochemistry, Kinetics, Atomic Charge, Solvation, Chemical Bonding	DFT, WFT, ELF, NBO, AIM, Solvation models	Julen Munárriz	UniOvi (QTCOVI)