

Institute/Department (if different exists)	Acronym	Group Leaders	Web Page
Departamento Química Física	EFME	Iñaki Tuñón/J. Javier Ruiz-Pernía/Antonio Francés	www.uv.es/efme
Institute of Molecular Science	QCEXVAL	Daniel Roca-Sanjuán	http://qcexval.uv.es/
Departamento Química Física	SISCON	Begoña Milián Medina	
Institute of Molecular Science (ICMol)	MolMatTC	Enrique Ortí/Juan Aragón/Joaquín Calbo	www.molmattc.com
Departamento Química Física		Lourdes Gracia	
Departamento Química Física	MOLPRO	Alfredo Sánchez / Inmaculada García	
METHODOLOGY			
General keyword	Details in topic	Researchers involved	Institute (Group Acronym)
Methodology Computational	Molecular Dynamics		
	Free Energy Methods		

Computational simulations of Biomolecules	QM/MM Methods	Inaki Luonon/J. Javier Ruiz-Poernía/Antonio Francés	EFME
Multiconfigurational quantum chemistry	Acceleration of photodynamics with Deep Learning / Spectroscopy, Photochemistry and Chemiexcitation in Condensed Phases	Daniel Roca-Sanjuán	QCEXVAL
Modelling Nonlinear Spectroscopy	QM/MM / Pump-probe / 2DES / Photoelectron / Resonance Raman	Javier Segarra-Martí	
Quantum Chemistry of Conjugated Systems	(TD)DFT	Begoña Milián Medina	SISCON
	Semiempirical Methods		
	QM/MM Methods		
	Ab Initio Methods		
Methodology for Charge/Exciton Transport in Molecular Aggregates	Multiscale Approaches (Electronic Structure Calculations / Model Hamiltonians / Quantum Dynamics)	Enrique Ortí/Juan Aragón/Joaquín Calbo	MolMatTC
Computational Modelling of Supramolecular Polymers	DFT / GFN2-xTB / MD		

Computational design of organic/inorganic conducting crystals	Periodic DFT calculations		
Computational simulations of oxide materials	Periodic DFT	Lourdes Gracia	
Ab initio methods for medium and large systems	CC/MP2	Alfredo Sánchez / Inmaculada García	MOLPROP

APPLICATIONS