

METHODOLOGY			
General keyword	Details in topic	Researchers involved	
Development of QM/MM methods	Development of a general QM/MM platform	Sergio Martí	
	Development of improved QM/MM techniques to explore free energy surfaces	Sergio Martí, Vicent Moliner	
Development of effective mass methods for nanocrystals	Interband coupling and single-particle potentials	Josep Planelles, Juan I. Climente	
	Few-body interactions	Josep Planelles, Juan I. Climente	
APPLICATIONS			
Systems	Property	Methods	Researchers involved
Computer assisted design of new inhibitors	cluster of CPUs with and without GPUs		Vicent Moliner, Sergio Martí, Raquel Castillo,
Computer assisted design of new biocatalists	cluster of CPUs with and without GPUs		

Computational study of enzyme catalyzed processes	cluster of CPUs with and without GPUs	QM/MM methods	Vicent Moliner, Sergio Martí, Katarzyna Swiderek, Miquel A. Galmés, Daria De Raffe
Theoretical and experimental studies on the relationship between non-molecular solid materials and their analogous molecular clusters	cluster of CPUs + MM lab + UFSC Lab		Juan Andrés, Mónica Oliva, Vicent S. Safont, Amanda Fernandes Gouveia, Marcelo de Assis, Eduardo de Oliveira Gomes, Iva Matteus Pinatti
Theoretical-experimental studies on (nano) solid materials with properties of industrial interest	cluster of CPUs + UFSC Lab		Juan Andrés, Mónica Oliva, Vicent S. Safont, Amanda Fernandes Gouveia, Marcelo de Assis, Eduardo de Oliveira Gomes, Iva Matteus Pinatti
Chemical structure and reactivity: bonding, reaction mechanisms and topological analysis of electron density	cluster of CPUs		Juan Andrés, Mónica Oliva, Vicent S. Safont
Design of solid materials with properties of industrial interest	cluster of CPUs + UFSC Lab		Juan Andrés, Amanda Fernandes Gouveia, Marcelo de Assis, Eduardo de Oliveira Gomes, Iva Matteus Pinatti
Behavior of solid materials under pressure: phase transitions	cluster of CPUs		Juan Andrés, Armando Beltrán
Semiconductor nanocrystals	Electronic structure, magnetism, spectroscopy	Effective mass theory	Jordi Llusar, David Macías-Pinilla, Josep Planelles, Juan I. Climente