TEAMS	TEAM LEADERS	E-mail	
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METHODOLODOGY			
Topic	**Method**	**People**	**Lab (group)**
		Aude Simon, Mathias Rapacioli, Martial Boggio-Pasqua, Nicolas Suaud, Arian Berger	
Methodology for strongly correlated systems, including relativistic effects	Model Hamiltonians for extended systems. Collective effects		LCPQ (SEM, THEO)
	Improvement of relativistic effects treatments for ZFS tensor and magneto-electric coupling		
	Periodic DFT, Green's Function, DMFT		
	(SC)2 dressings of IC, MRCC or perturbative methods		
	Improvement of DFT descriptions for highly correlated systems (Spin decontamination, spin polarization…)		

Systems	Methods		People / Lab
Approximate DFT, periodic and non-periodic, large and extended systems	DFTB		LCPQ (MAD)
Periodic systems	WFT, DFT, QMC, MBPT, Clifford Boudary Conditions for the ab initio treatment of periodic systems, Model Hamiltonians		LCPQ (SEM, THEO)
Excited-state properties	Selected CI (CIPSI), coupled cluster, DFT (TDDFT, ensemble DFT), MBPT (GW, BSE)		

APPLICATIONS				
Systems	**Property**	**Methods**	**People**	**Lab (group)**
Transition metal oxyde materials; transition metal, lanthanides and actinides complexes (organic or inorganic ligands)	Spectroscopy, Magnetism, Spin-orbit and Hyperfine Interactions, High-Tc superconductivity, Disorder, Phase transitions	WFT, DMFT, DFT / Embedded Fragments / Model and Effective Hamiltonians		LCPQ (MAD, PHOTOTEC, SEM, THEO)

Conjugated hydrocarbon systems, PAH, astrochemical applications	Geometry, Spectroscopy, Magnetism, Aromaticity, Bistability, Dynamics, Photophysics, Reactivity	WFT, DFT, SF-DFT, TD-DFT, DFTB, CC / Model Hamiltonians		LCPQ (MAD, SEM, THEO, PHOTOTEC)
Clusters (metal, noble gaz, covalent, molecular, astrophysically relevant), Condensed phase (water, gas hydrates)	Geometry, spectroscopy, dynamics, reactivity, fragmentation, collision	WFT, CC, DFTB, QM/MM, Molecular Dynamics		LCPQ (MAD, THEO)
Organic molecules	Soil interactions; pesticides	WFT, DFT, TD-DFT, SD-DFT, Molecular Dynamics, DFTB		LCPQ (MAD, PHOTOTEC, SEM)
	Optical and redox properties, photochromism, photoreactivity, Magnetism			
Wigner crystal	Electronic properties	WFT, ad hoc codes		LCPQ (THEO)

Diatomic molecules containing ionic states. Astrophysics.	Spectral profile, diabatization,metastable states, vibronic effects	WFT, DVR		LCPQ (THEO)
Particles, nuclei, atoms and small molecules	Parity non-conservation, symmetry violation beyond the Standard Model	General many-body methods		LCPQ (THEO)