Institute/Department (if different exists)	Acronym	Group Leaders	Web Page
		director: Jean Philip PIQUEMAL	https://www.lct.jussieu.fr/?page_id=78
LCT Laboratoire de Chimie Théorique	Theme 1: Electronic structure methods	Julien TOULOUSE	https://www.lct.jussieu.fr/?page_id=368
LCT Laboratoire de Chimie Théorique	Theme 2: chemical interpretation	Julia CONTRERAS-GARCIA	https://www.lct.jussieu.fr/?page_id=591

LCT Laboratoire de Chimie Théorique	Theme 3: Dynamical simulations: structure and reactivity	Riccardo SPEZIA	https://www.lct.jussieu.fr/?page_id=469
LCT Laboratoire de Chimie Théorique	Theme 4: Extreme Scale Mathematically-Based Computational Chemistry	Jean-Philip PIQUEMAL	https://www.lct.jussieu.fr/?page_id=831
LCT Laboratoire de Chimie Théorique	Theme 5: Organic, organometallic and inorganic chemistry	Hélène GERARD	https://www.lct.jussieu.fr/?page_id=376
LCT Laboratoire de Chimie Théorique	Theme 6: Chemistry in space: from MIS to Earth	Alexis MARKOVITS	https://www.lct.jussieu.fr/?page_id=495
LCT Laboratoire de Chimie Théorique	Theme 7: Materials for Environment and Energy	Monica CALATAYUD	https://www.lct.jussieu.fr/?page_id=567

METHODOLODOGY			
General keyword	**Details in topic/Keywords**	**Researchers involved**	**Institute (Group Acronym)**
Theme 1: Electronic structure methods	Development of methods based on density-functional theory and wave-function theory	Julien TOULOUSE, Emmanuel GINER, Eleonora LUPPI, Peter REINHARDT	LCT
	Development of methods based on localized orbitals	Peter REINHARDT, Benoit BRAIDA, Emmanuel GINER	LCT
	Development of quantum Monte Carlo methods	Roland ASSARAF, Benoit BRAIDA, Emmanuel GINER, Julien TOULOUSE	LCT
	Development of methods for spectroscopy and electron dynamics	Eleonora LUPPI, Roland ASSARAF, Julien TOULOUSE	LCT

	Method developement in Valence Bond Theory	Benoît Braïda	LCT
Theme 2: chemical interpretation	Application of Valence Bond theory to chemical bonding	Benoît Braïda	LCT
Theme 3: Dynamical simulations: structure and reactivity	Chemical reactivity under vibrational strong coupling. DFTB, ReaxFF, Path Integral.(ANR funding one M2 studentship in 2021-2022)	R.Spezia, J.Richardi	LCT
	Nuclear quantum effects for ion-molecule gas phase reactions. Ring Polymer MD, Quantum Thermal Bath.(possible funding COST CA18212 – Molecular Dynamics in the Gas Phase)	R.Spezia	LCT
Theme 4: Extreme Scale Mathematically-Based Computational Chemistry			LCT

APPLICATIONS				
Systems	**Property**	**Methods**	**Researchers involved**	**Insitiute (Group Acronym)**
Theme 5: Organic, organometallic and inorganic chemistry	geometric and electronic structure, energetics, physico-chemical caracterization, reactivity	quantum-chemical molecular electronic-structure (gaz phase and solvent). In close collaboration with experimental teams.	I. Chataigner, G. Frison, H. Gérard, S. Halbert, O. Parisel	LCT
Homogeneous Catalysis	Multi-step reaction pathways, selectivity	DFT (gaz phase and solvent), AIMD	I. Chataigner, G. Frison, H. Gérard, S. Halbert, O. Parisel	LCT
Open-shell systems	Electron transfer, spin densities, reactivity	DFT, TD-DFT, post-HF methods	I. Chataigner, G. Frison, H. Gérard, S. Halbert, O. Parisel	LCT
Elusive species	Structure and physico-chemical characterization	interpretative methods for electronic structure description	I. Chataigner, G. Frison, H. Gérard, S. Halbert, O. Parisel	LCT

Theme 6: Chemistry in space: from interstellar medium to Earth	Molecular complexification in rarefied gas phase: geometry, energetics, chemical reactivity (ion-molecule and neutral-neutral reactions).	DFT and post-HF calculations (Gaussian)	Isabelle Fourré	LCT
	Complex Organic Molecules in the Insterstellar Medium, prebiotic chemistry, Surface Chemistry, heterogeneous catalysis with grains (solids, ices)	Periodic DFT (VASP, CRYSTAL), DFT and post-HF calculations (Gaussian)	A. Markovits, F. Volatron, F. Fuster, F. Fuster	LCT
Theme 7: Materials for Environment and Energy	Surfaces, interfaces and nanoparticles: geometry, energetics, spectroscopy, chemical reactivity of bulk, surfaces, nanoparticles, gas-phase inorganic crystals. Metals, CeO2, TiO2, H2 adsorption systems	periodic DFT (VASP, Crystal), AIMD	M. Calatayud	LCT

Finally indicate below possible ways to raise fundings to support mobility periods for students going to you institution (European COST Actions, local and/or national fundings, collaborative projects…)

French ANR funding one M2 studentship in 2021-2022	Theme 3, Riccardo Spezia
COST CA18212 – Molecular Dynamics in the Gas Phase	Theme 3, Riccardo Spezia
ANR RHOCKI (funding for M2 internship)	Theme 5: Mechanistic studies of the Hock rearrangement
Institut de science des matériaux (IMat) (funding for M2 internship + mobility)	Theme 5: Structure and electronic properties of realistic copper clusters in solution

COST CA18234 - Computational materials sciences for efficient water splitting with nanocrystals from abundant elements	Theme 7: static and dynamic computation of nanocystals: reactivity, energetics, spectroscopy
RIA Nanoinformatix	Theme 7: Computational modelling of nanotoxicity
RIA CHARISMA	Theme 7: computing Raman spectra, scripting, databases, web interface