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.	R.Spezia, J.Richardi	LCT
	(ANR funding one M2 studentship in 2021-2022)		
	Nuclear quantum effects for ion-molecule gas phase reactions. Ring Polymer MD, Quantum Thermal Bath.	R.Spezia	LCT
	(possible funding COST CA18212 – Molecular Dynamics in the Gas Phase)		
APPLICATIONS			
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