KU LEUVEN

Researchers involved	Systems
Professor Liviu CIBOTARU	Theoretical and computational study of magnetism in molecules and materia
Professor Daniel ESCUDERO	Quantum chemical modeling of the excited states, photophysical and photochemical properties of molecular systems
	Developments of excited state decay rate formalisms and computational protocols for quantitative determinations of photochemical properties. We are also interested in the development of descriptors for photochemical reactivity
	Modeling organic electronics: OLEDs and thermoelectrics
	Modelling organometallic chemistry and mechanisms of catalysis with DFT and post-HF methods
Professor Jeremy HARVEY	Biomolecular energy landscapes and reactivity, probed through the use of molecular dynamics simulation and analysis thereof, as well as through hybrid quantum mechanical and molecular mechanical (QM/MM) methods. We also are involved in development of QM/MM methodology

	Organometallic chemistry and mechanisms of catalysis, studied using especially density functional theory quantum chemical methods.
	Chemical reactivity in condensed phases, studied using molecular dynamics and quantum chemical methods
	Molecular self-assembly, studied using molecular dynamics and mechanics as well as (periodic) quantum chemical methods.
	Gas-phase and especially atmospheric chemistry reaction mechanisms, studied using quantum-chemical methods
Professor Thomas JAGAU	Theory of electronic resonances & non-Hermitian quantum chemistry.
	Development of coupled-cluster and equation-of-motion coupled-cluster methods
	Reaction mechanisms in electrochemistry
	(Theoretical) photoelectron spectroscopy
Professor Jérȯme LOREAU	Collisional ro-vibrational excitation of molecules in astrophysical environments by means of quantum-mechanical and semi-classical methods. All calculations make use of high-level ab initio potential energy surfaces.
	Chemical reactivity at low temperature. We investigate gas-phase processes involving small molecules (less than 10 atoms) with different methods (quantum-mechanical, semi-classical, statistical) with the aim of understanding their reaction properties. We apply our calculations to astrochemistry models or to help interpreting cold chemistry experiments.
	Spectroscopy of weakly-bound molecular complexes. We use quantum-mechanical techniques to obtain microwave or infrared spectra of molecules bound by weak forces such as van der Waals interactions that can be compared to experiments.