UNIVERSITAT DE BARCELONA

Research Group	Institution	Group Leader	Other researchers *	Development or application of	Active research lines **	Methodologies
Applied Computational Chemistry & Molecular Modelling (ACC&MM)	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. Ramón Sayós (r.sayos@ub.edu)	Dr. Pablo Gamallo (gamallo@ub.edu) Dr. Fermin Huarte (fermin.huarte@ub.edu)	Application	* Capture and gas separation * Heterogeneous catalysis for CO2 conversion	* Density functional theory (DFT) * Molecular dynamics (MD) * Grand canonical Monte Carlo (GCMC) * Kinetic Monte Carlo (kMC) * Microkinetic modelling

Electronic Structure Group	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. Eliseo Ruiz (eliseo.ruiz@qi.ub.edu) & Prof. Pere Alemany (p.alemany@ub.edu)	Prof. Gabriel Aullón (gabriel.aullon@qi.ub.edu) Dr. Jordi Cirera (jordi.cirera@qi.ub.edu) Dr. Jorge Echeverria (jorge.echeverria@qi.ub.edu) Dr. Silvia Gómez-Coca (silvia.gomez@qi.ub.edu) Dr. Jesús Jover (jesus.jover@qi.ub.edu) & Dr. Miquel Llunell (llunell@ub.edu)	Application & Development	* Molecular magnetism * Single-molecule transport devices * Organometallic chemistry and reactivity * Weak interactions * 2D materials & * Continuous symmetry measures * Electronic transport and magnetism in low dimensional solids * Crystal packing in molecular solids	* Density functional theory (DFT) * Post Hartree-Fock methods * Topics magnetism and transport also experimental studies combined with theory & * Molecular dynamics * Continuous symmetry measures
Computational Photobiology Lab (CPL)	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. Carles Curutchet (carles.curutchet@ub.edu)	------	Application & Development	* Photosynthetic light harvesting * Spectroscopy and energy transfer in biomolecules	* Molecular dynamics * Polarizable QM/MM and continuum solvation models * Time-dependent density functional theory (TD-DFT) * Lineshape theory for optical spectra

Computational Materials Science Laboratory (CMSL)	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. Francesc Illas (francesc.illas@ub.edu)	Prof. Carme Sousa (c.sousa@ub.edu) Dr. Ramon Costa (rcosta.ub.edu) Dr. Francesc Viñes (francesc.vines@ub.edu) Prof. Konstantin M. Neyman (konstantin.neyman@icrea.cat) Dr. Stefan T. Bromley (s.bromley@ub.edu) Dr. Ángel Morales García (angel.morales@ub.edu). Dr. Albert Bruix (abruix@ub.edu)	Application	* Heterogeneous catalysis * Photocatalysis * Nanotechnology * 2D Materials * Modeling nanostructured materials and interfaces for energy-related applications * Computational characterization of catalysts under reaction conditions * Development of structure prediction approaches assisted by machine learning	* Density functional theory (DFT) * Time-dependent DFT (TDDFT) * Ab Initio thermodynamics * Kinetic Monte Carlo (kMC) * Microkinetic modeling * Monte Carlo Simulations * Electronic structure * Characterization methods * Machine Learning * Structure prediction algorithms
Computational Electrocatalysis Group	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Dr. Federico Calle-Vallejo (f.calle.vallejo@ub.edu)	Dr. Manuel Kolb (mjkolb@ub.edu)	Application	* CO2 electroreduction * Nitrogen cycle electrocatalysis * Fuel cells * Electrolyzers	* Density functional theory (DFT) * Microkinetic modelling * Semiempirical modelling

Molecular Materials Structure Group (GEM2)	Materials Science and Physical Chemistry Dept. & Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. Mercè Deumal (merce.deumal@ub.edu)	Prof. Juan J. Novoa (juan.novoa@ub.edu) Dr. Jordi Ribas Ariño (j.ribas@ub.edu)	Application	* Physical properties of molecular multifunctional materials (magnetism, conductivity) * Spin-crossover materials * Phase transitions in molecule-based materials	* Multiscale modeling * DFT and wave-function based methods * Periodic methods * Molecular dynamics * Statistical mechanics * Machine learning
Modelling of Biological Systems and Drug Design	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. Jaime Rubio (jaime.rubio@ub.edu)	------	Application & Development	* Drug Design	* Docking * Molecular dynamics
Quantum simulation of Biological Processes	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. Carme Rovira (c.rovira@ub.edu)	------	Application	* Enzyme catalysis	* Density functional theory (DFT) * Molecular dynamics * QM/MM MD * Metadynamics * Docking
Theoretical and Computational Organic and Bioorganic Chemistry	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Dr. Josep Maria Bofill Villà (jmbofill@ub.edu)	Dr. Jordi Poater Teixidor (jordi.poater@ub.edu)	Application & Development	* Non-covalent interactions * Biradicals	* Density functional theory (DFT)

Computational Biology, Chemistry and Gastronomy (CBCG)	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. F. Javier Luque (fjluque@ub.edu)	Dr. C. Estarellas (cestarellas@ub.edu) Dr. Salomé Llabrés (salome.llabres@ub.edu) Dr. A. Bidon-Chanal (abidonchanal@ub.edu)	Application & Development	* Molecular recognition and binding * Enzyme allostery * Drug design * Computational gastronomy	* Quantum chemical calculations * Molecular dynamics simulations * Enhanced sampling techniques * Computer-aided drug design * Chemoinformatics
Reaction Dynamics and Complex Systems	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Prof. Miguel González (miguel.gonzalez@ub.edu)	------	Application & Development	* Reaction dynamics in gas phase * Reaction and energy transfer dynamics in superfluid helium nanodroplets	* Ab initio calculations on potential energy surfaces * Quantum Dynamics * Quasiclassical dynamics

Biophysical Chemistry of Macromolecules and Colloids (BioPhysChem)	Institute of Theoretical and Computational Chemistry (IQTC , Universitat de Barcelona)	Dr. Sergio Madurga (s.madurga@ub.edu)	Prof. Francesc Mas (fmas@ub.edu)	Application & Development	* Effect of polyelectrolyte interaction in the contaminant adsorption onto microplastics in natural waters. * Effect of macromolecular crowding in enzymatic processes of cellular metabolism *Modeling of processes with Intrinsic Disordered Proteins (IDPs)	* Constant pH simulations. * Semi and Grand Canonical Monte Carlo (SGCMC & GCMC) * Langevin dynamics * Molecular dynamics