

**RESEARCH GROUPS INVOLVED IN THE MASTER'S THESES OF THE  
Master's Degree in Atomistic and Multiscale Computational Modeling in  
Physics, Chemistry and Biochemistry**

**Participating Organisms (BKC)**

**Facultat de Química (UB) (coordination)**

- **Departament de Química Física**
  - **Biophysicalchemistry of Macromolecules and Colloids (BioPhysChem)**  
Macromolecular Crowding; Reaction-Diffusion Processes in Gels and Intracellular Media; Macromolecular Complexation; Polyelectrolytes; Soft Nanoparticles; Colloids; Monte Carlo, Molecular Dynamics; Brownian Dynamics  
<http://www.ub.edu/biophyschem/>
  - **Molecular Dynamics of Biomembranes**  
Biophysics, Cell Membrane, Cell Signaling, Molecular Dynamics  
<http://www.ub.edu/socsam/cms/index.php/research-top/biophysics>
  - **Molecular Materials Structure Group**  
Molecular magnetism, Crystal packing, Spin transitions, Phase transitions, Bistability  
<http://www.ub.edu/gem2/welcome.html>
  - **Reaction Dynamics Group**  
Quantum Dynamics, Reactivity, Molecular Dynamics, Gas storage  
<http://www.ub.edu/gdrq>
  - **Surface Chemistry and Catalysis**  
<http://www.ub.edu/cmsl/cmsl/research/surface-chemistry.html>
- **Departament de Química Orgànica**
  - **Quantum simulation of biological processes**  
Quantum mechanics/molecular mechanics (QM/MM), Ab initio molecular dynamics, Enhanced-sampling, Glycobiology, Enzyme catalysis  
<http://www.icrea.cat/Web/ScientificStaff/Carme-Rovira-Virgili-411>

**Facultat de Física (UB)**

- **-Departament de Física Fonamental**
  - **Group of Statistical Physics**  
Nonequilibrium Statistical Mechanics; Physics of Viruses; Water and Anomalous Liquids; Radiative energy exchange at the nanoscale; Irreversible deformation below the microscale  
<http://www.ffn.ub.edu/statphysgroup/>
  - **Soft Matter Physics Group**  
Mesoscopic modeling, nonequilibrium statistical physics, active matter, granular fluids, complex fluids  
<http://www.ignasipagonabarraga.eu/>
- **Departament d'Estructura i Constituents de la matèria**
  - **-Materials: phase transitions and multiscale systems**  
Structural and magnetic transitions in materials, caloric and multicaloric effects, hysteresis, metastability and avalanche response.  
[http://www.ub.edu/web/ub/en/recerca\\_innovacio/recerca\\_a\\_la\\_UB/grups/fitxa/M/MATEFASE/index.html](http://www.ub.edu/web/ub/en/recerca_innovacio/recerca_a_la_UB/grups/fitxa/M/MATEFASE/index.html)

## **Spatio temporal order in biophysical systems under fluctuations**

<http://www.ecm.ub.es/~jmsancho/>

### **Facultat de Biologia (UB)**

- **Departament de Bioquímica i Biologia Molecular**

### **Facultat d'Informàtica (UPC)**

- **Barcelona Quantum Monte Carlo Group**  
Our goal is the study of quantum fluids and solids using an ab initio approach based on Quantum Monte Carlo methods. We work on the development of new algorithms for simulation of fully quantum systems and apply these methods to a variety of systems, ranging from dilute cold Bose and Fermi gases to more strongly correlated systems, such as Helium and molecular Hydrogen.  
[bqmc.upc.edu](http://bqmc.upc.edu)
- **Computer Simulation in Condensed Matter Research Group (SIMCON)**  
Molecular Liquids and Solutions, Quantum Matter, Complex Networks, Molecular Dynamics, Quantum Monte Carlo  
[simcon.upc.edu](http://simcon.upc.edu)

### **Escola Tècnica Superior d'Enginyeria Industrial (UPC)**

- **Innovative Materials and Molecular Engineering (IMEM)**  
Nanostructures and nanodevices based upon synthetic and natural polymers  
<http://recerca.upc.edu/imem/index.htm>
- **Non-Linear Physics and Out of Equilibrium (NOLIN)**  
Cell Biophysics; Computational neuroscience; Complex fluids; Chemical reaction-diffusion systems; Superconductivity  
<http://nolin.upc.edu/en>

### **Institut de Química Avançada de Catalunya (CSIC)**

### **Barcelona Supercomputing Center (BSC)**

- **EAPM: Atomic and Electronic Protein Modelling**  
QM/MM and Monte Carlo studies of complex biochemical processes. We center on enzyme engineering and substrate/drug binding.  
<http://www.bsc.es/life-sciences/electronic-and-atomic-protein-modelling>