Molecular Modeling and quantum Mechanical Methodology
dealing with Nature at the Nanoscale

http://iqc.udg.edu/m4/
Institute of Computational Chemistry

• **Members**
  – permanent:
    • three full professors
    • five associate professors
    • one ICREA senior
  – post-docs:
    • one ICREA Júnior
    • two Ramón y Cajal
    • one Beatriu de Pinós
  – graduate students: 13
  – undergraduates: 3
  – project manager
  – secretary
  – informatician

• **Output**
  – ISI publications ’06-’08: >200
  – five projects MICINN, I+D+i
  – several projects MareNostrum supercomputer, Barcelona
  – organization Researcher’s Night (FP7)
  – bi-annual conference:
    • 2006 chemical bond
    • 2008 aromaticity
    • 2010 electron density, density matrices and density functional theory
  – collaborations with industry and public entities
    • Ciba, Lucta, Leitat
    • Hospital Josep Trueta

• **Consolidated group (SGR)**
Computational resources

- In-house clusters

- External clusters

MareNostrum cluster, BSC
Main research lines M4

• Aromaticity and reactivity studies
• Peptides and molecular interactions
• Modelling photochemistry
• Bioinorganic chemistry and biomedicine
• Electron transfer in biomolecules and organic materials
• Nonlinear optical properties
• Organometallic hydrides
• Method development
Nonlinear optical properties

- **Nonlinear optics (NLO)** studies the interaction between matter and rays of light of very high intensity.
- Only laser-light is sufficiently intense to produce NLO effects, therefore: NLO phenomena are not observed in Nature.

Applications of nonlinear optics: laser technology, telecommunications (fiber optics), informatics and other new technologies

\[ P_{tot} = P_{el} + P_{vib} \]

- **Electronic contribution** \((P_{el})\): perturbation of electron cloud
- **Vibrational contr.** \((P_{vib})\): perturbation of nuclear positions and PES curvature
Electron Transfer in Biomolecules and Organic Materials

• **Development of semiempirical schemes**
  - Large models for bio- and nano-systems
  - Averaging electronic properties over large time scales
  - Spectroscopic properties of large chromophores

• **QM/MD calculations**
  - Generating MD trajectory
  - QM calculations of electronic structure
  - Estimation of key parameters that control the ET rate
  - Quantitative analysis of ET and electrical conductivity

\[ k = \frac{2\pi V_{DA}^2}{\hbar} \frac{1}{\sqrt{4\pi \lambda kT}} \exp \left[ -\frac{\left(\Delta G + \lambda \right)^2}{4\lambda kT} \right] \]

• **Design of molecular devices**
  - Tuning geometry of elements and their arrangement
  - Role of coordinated transition metals
  - Photoinduced charge separation in solar cell modes
  - Efficient bridges between electron donor and acceptor

Damage and repair of DNA due to ET

Strong effects of structural dynamics

Dr. A. Voityuk
Reaction mechanisms, aromaticity and chemical bonding

- **Mechanistic studies** with localization of intermediates and transition states in organic chemistry (fullerenes), organometallic and bioinorganic chemistry

- Studies of **aromaticity**. Determination of new aromaticity indices based on study of electronic delocalization in molecules. Application to metallic clusters

- Nature of the **chemical bond**. Studies of decomposition of the energy. Analysis of AIM and ELF
DNA replication, aromaticity and molecular imaging

• **Theoretical analysis of aromaticity** by means of electronic-based criteria
  – Application of para-Delocalization Index (PDI), measure of electronic delocalization, to polycyclic aromatic hydrocarbons and fullerenes, reactivity analysis,…

• **DNA replication mechanism**, taking into analysis steric shape, hydrogen bonds, π-stacking and solvent effect for its selectivity
  – Base pair dimers and trimers as models

• Development of **new contrast agents** to improve molecular imaging in brain ictus (in collaboration with neurology and radiology departments in Hospital Trueta)
Transition metal silyl hydrides and bimetallic polyhydrides

Hydrogen exchange in CpRu(µ-H)₄RuCp

CpRh(SiMe₃)₃H

TS:
ΔE‡ = 2.6 kcal mol⁻¹
ΔG‡ = 1.9 kcal mol⁻¹

J (Si-H):
-8 Hz (calcd. average)
-13 Hz (expt.)

Mayer bond indices:
0.18/0.14

Dr. S. Vyboishchikov
(Bio)inorganic chemistry and biomedicine

- Chemical bonding and reactivity in DNA and transition-metal complexes

- Method development: multi-level (QM/MM, QM/QM) schemes

- Application to (bio)chemical systems
Excited states and non-adiabatic processes

- Molecular photochemistry and photophysics
- Light – molecule interaction
- Interpretation of ultrafast laser spectra (UV, vis)
- Applications of biological and technological interest:
  - Methodologies to characterize the relevant features of the potential energy surface (conical intersections)
Hydrogen bond, dihydrogen bond & aminoacid radical cation

• **Hydrogen bond**: Resonance assisted hydrogen bond

• **Dihydrogen bond**

• **Aminoacid Radical Cation Studies**: Characterization and reactivity

**Histidine radical cation**

Dr. S. Simon
Molecular dynamics simulation of antimicrobial peptides and their mechanism of action

Specific hydrogen bond

Lys$^2$-Phe$^6$
Leu$^3$-Phe$^6$

Lys$^4$-Lys$^5$

β-turn

Conformation of a ten residue cyclic peptide

Model for cooperative action

Pore formation on a DPPG membrane model

Trajectory analysis

Dr. P. Salvador

Institut de Química Computacional
What can we do

• Simulation of electronic spectra (UV, Vis, NMR) of molecules and materials

• Detailed information of reaction mechanisms
  – influence of metal ions

• Determination of physico-chemical properties
  – NLO, aromaticity, ..

• Understanding chemistry in terms of physical concepts
  – photophysics, chemical bonding, ..
People

M. Duran  M. Solà  A. Voityuk  S. Simon  Ll. Blancafort

S. Vyboishchikov  J. Poater  J.M. Luis  P. Salvador  M. Swart