

Theory days

Biomolecule irradiation

Dec 2, 3, 4, 2009

IRSAMC

Toulouse

Collisional/laser irradiation
Ab initio methods
Time dependent DFT
Direct/indirect mechanisms
Effects of solvent
...



dépasser les frontières

GdR
DFT++



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THEORY DAYS ON BIOMOLECULE IRRADIATION

1 Aim and scope

The aim of the meeting is to put together theorists interested in the modelling of irradiation processes in molecules of biological interests. There are presently complementing efforts by physicists and chemists on such topics. Highly elaborate quantum chemical methods allow the mostly static description of large biological molecules possibly in contact with a solvent. On the other hand, effective theories such as Density Functional Theory are now practically available in the time domain and allow to follow explicitly in time both excitation and response of an irradiated system, at least in the case of simple bio-molecules. A key issue is thus to try to establish firm links between such complementing approaches, for example by the joined analysis of intermediate size model systems.

We plan to gather people from the various groups working in this domain in western Europe. The workshop is intended to be a working forum, thus rather informal. The format will consist in a series of long detailed talks, typically 1 hour (40 mn talk + 20 mn for questions) focusing in particular on ongoing problems and open ends. Some free time will furthermore be reserved for collective discussions. We thus urge participants to prepare their talks in this spirit. Ultimately a most efficient organization would consist in having a limited number of talks per representative group in order to avoid doublings.

A somewhat similar initiative is currently being developed in far East Asia (China, Japan, Korea) and contacts are established with some of these groups. Some representatives of Asia will also join the meeting. If a consensus is reached during the workshop it would be highly profitable to envision a sequel to this workshop in order to possibly establish, at best collaborative links between the various groups with possible exchange of researchers and students, at worst an ongoing follow up of progress in the field.

Several initiatives are presently under discussion in Europe to gather the scientific community around the problems of irradiation of biomolecules. The present project is dedicated to theorists and thus not in competition with these larger scope projects. On the other hand a successful gathering of the theory community might constitute a valuable support for these projects. A first step in this direction was already achieved late 2007 with the Frejus workshop organized in the framework of the former RADAM Cost P9 program. We now want to pursue the efforts in this direction.

2 Scientific program

The detailed program will be prepared as soon as possible after replies from participants. We plan to start the workshop on Wednesday Dec 2 just after lunch and end it on Friday Dec 4 early afternoon. This would allow participants to reach Toulouse in the morning of Dec 2 and be back home in the evening of Dec 4.

A tentative program is thus :

Dec 2 : 14:00 - 17:30 (3 × 1 hour + 1 coffee break)

Dec 3 : 08:30 - 13:00 (4 × 1 hour + 1 coffee break)

Dec 3 : 14:30 - 18:00 (3 × 1 hour + 1 coffee break)

Dec 4 : 08:30 - 13:00 (4 × 1 hour + 1 coffee break)

Dec 4 : possibly a short final session in the afternoon.

3 Practical aspects

3.1 Registration and lodging

There will be no registration fee. We shall cover lodging, meals, and local transportation for about 15 participants during the duration of the workshop (arrival Dec 2, departure Dec 4), on the basis of first confirmed, first served.

Participants will be lodged in hotels downtown Toulouse at walking distance from major metro stations along line B. There is a direct metro line (line B) connecting downtown to university. Travel takes about 20 minutes with trains every few minutes (less than 5 mn).

Meeting will take place at IRSAMC in the university Campus : for a map, see <http://www.irsamc.ups-tlse.fr/index.php?lien=venir>

3.2 Access to Toulouse

Airports

Toulouse airport is connected to major west European airports and hubs (Paris Orly and Roissy Charles de Gaulle, Munich, Frankfurt, London, Amsterdam) with regular connections by Air France/KLM, Lufthansa, British Airways for the major companies and also with connections by (Low Cost) Easy Jet. Plane provides by far the simplest access to Toulouse with reasonable fees for sufficiently early booking.

<http://www.toulouse.aeroport.fr/>

There is a shuttle to downtown (first stop at Compans Caffarelli, on line B of metro) every 20 mn (cost is 4 euros one way, 6.3 euros return trip); for details, see

<http://www.toulouse.aeroport.fr/fr/aeroport/acces-plans-parkings/acces/se-deplacer-en-transport-en-commun>

As soon as one catches the shuttle, it takes about half an hour to get to the University thanks to the connection with line B at Compans Caffarelli station.

An alternative access is provided by Carcassonne airport (about 45 minutes by car from Toulouse) which has a Low Cost access through Ryanair

<http://www.carcassonne.aeroport.fr/>

In case of major problem, we shall organize some transfer. It would be useful to know sufficiently in advance such details.

Train

Central station is Toulouse Matabiau connected to line A of metro (see below) and is connected to major french cities.

<http://www.gares-en-mouvement.com/gare-fr-1-frxyt.html>

Metro

Metro and bus connections (general): <http://www.tisseo-urbain.fr/horaires/>

line A (train station to downtown): <http://www.tisseo-urbain.fr/734991.pdf>

line B (downtown to university): <http://www.tisseo-urbain.fr/734994.pdf>