

Application for Faculty Grant for International Connections

A. Peet Hickman

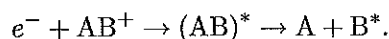
Department of Physics, Lehigh University, Bethlehem, PA 18015

Summary

Hosts	Dr. Fabien Gatti and Dr. Dahbia Talbi Université de Montpellier II, 34095 Montpellier, France
Time of visit	two weeks in June, 2010
Purpose of visit	to meet Dr. Gatti for the first time and plan work on future projects
Estimated total cost	\$2500

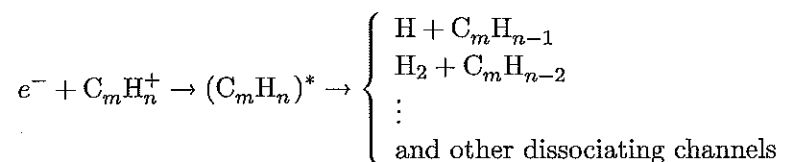
Rationale for the Visit, Goals, and Expected Results

For the past few years, part of my research has involved a collaboration with Dr. Dahbia Talbi of the University of Montpellier [1, 2]. We have performed calculations related to modeling a molecular process known as Dissociative Recombination (DR), which is the electronic analog of a chemical reaction. A simple, schematic example of this process is the following:



The electron combines with the diatomic molecular ion AB^{+} to form an excited neutral system $(AB)^{*}$, which then breaks up into fragments. Some of the fragments may be in excited states (denoted B^{*}).

In many important applications, the initial molecular ion is larger, consisting of three, four, or more atoms. Calculations are then much more difficult. Several different sets of final products ("channels") are possible, and the "branching ratio" for each channel must be determined. For example, the DR of electrons with a hydrocarbon target can be written as



Dr. Talbi and I have submitted proposals to DoE and to NASA addressing problems of this type. DoE is interested because DR reactions involving hydrocarbons take place near the carbon walls of tokamak fusion plasmas. Similar reactions are important in the chemistry of the atmosphere of Saturn's satellite Titan. The reviewers of our proposals have suggested that we need a better method of treating the dynamics of the atomic motion after the electron capture. Dr. Talbi was aware of the work of her colleague Dr. Gatti in that area, and so we began discussions with him about a collaboration.

Dr. Gatti is one of the developers of a new and powerful method of modeling chemical reactions by calculating the possible trajectories of the atoms involved using quantum mechanical wave packets [3]. This method can be applied to the DR problem. We have begun a collaboration that has involved many email exchanges and a joint proposal, but we have not had a chance to meet in person and discuss our work in depth. Support for my visit to Dr. Gatti's laboratory would enable us to hold intensive discussions about how we can best combine forces and would lead to much stronger proposals for future work together.

In order to prepare for a visit, I am learning more about Dr. Gatti's work. One of my graduate students has started using Dr. Gatti's computer code and has performed several preliminary calculations. We have gained a general understanding of the capability of his code, but we have many questions about the details of applying it to DR. These preparations will ensure that Dr. Gatti and I can have productive discussions during a visit.

The professional goals of the trip are to meet Dr. Gatti, to learn more about the method he has developed, and to formulate problems that we can address together. During the visit I should be able to complete "proof of principle" calculations that will confirm the applicability of Dr. Gatti's method to DR. On the personal side, another goal of the visit is to take advantage of the opportunity to practice my French. In 1980–81 I lived in Paris and worked at the Centre d'Etude Nucléaire de Saclay for a year, and at that time I was able to carry on everyday conversations and discuss my technical work in French.

This proposed visit should lead to a much clearer vision of the future direction of our joint project. Based on the discussions in Montpellier, I will undoubtedly make some adjustments in the work with my graduate student. In the short run, this ongoing work will provide the foundation for future collaborative proposals. In the long run, Dr. Gatti, Dr. Talbi, and I should be able to combine our complementary areas of expertise and address many significant scientific problems in fusion technology and planetary atmospheres. Such work will enhance Lehigh's international visibility and recognition. It is also likely to lead to opportunities for the exchange of graduate students.

Arrangements in Montpellier

My hosts will try to arrange lodging in the International House at the University of Montpellier. If that is not possible, they will seek a hotel or short-term apartment rental near the campus. Depending on the accomodation, it may be necessary to eat most meals out. Office space near Dr. Gatti and Dr. Talbi and suitable computer connections for visitors are available.

Budget

I estimate €200 per week for lodging and €20 per day for food. Total living expenses for two weeks would be €680 (about \$950). Roundtrip airfare from Newark airport to Montpellier is about \$1383 (best price on travelocity.com on March 29, 2010). Other items such as bus service to and from Newark airport, checked baggage fees, and miscellaneous contingencies might account for another \$150. The total cost should be about \$2500.

Letters of Invitation

Letters of invitation from Dr. Gatti and Dr. Talbi are appended.

References

- [1] A. P. Hickman, R. D. Miles, C. Hayden, and D. Talbi, "Dissociative recombination of $e + \text{HCNH}^+$: Diabatic potential curves and dynamics calculations", *Astron. and Astrophys.* **438**, 31–37 (2005).
- [2] D. Talbi, A. P. Hickman, D. Kashinski, R. F. Malenda, and P. Redondo, "A comparative study of the DR reactions of $c\text{-C}_3\text{H}_3^+$ and $l\text{-C}_3\text{H}_3^+$: Preliminary theoretical studies", *Journal of Physics: Conference Series* **192**, 012014 (6 pages) (2009).
- [3] *Multidimensional Quantum Mechanics: MCTDH Theory and Applications*, edited by H.-D. Meyer, F. Gatti, and G. A. Worth (Wiley-VCH, Weinheim, 2009).

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Montpellier, March 26, 2010

Department of Physics,
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To the Foreign Travel Grant Committee:

I am a theoretical chemist in the field of quantum dynamics. I am research associate professor in the group of theoretical chemistry headed by O. Eisenstein in Montpellier, France.

Since several years, I have been interested in collaborating with my colleague Dr. Dahbia Talbi who is working in another department of the Montpellier University. I am aware of the importance of the Dissociative Recombination (DR) processes and I would appreciate very much to take advantage of the experience of Dr. Talbi and of her collaborator Pr. Peet Hickman in this field. We have already begun a collaboration with them involving many discussions with Dr. Tahbi, email exchanges and a local joint proposal. In particular, Pr. Hickman has started to learn how to use the MCTDH package but it would be much more efficient if I could meet Pr. Hickman to directly work with him and Dr. Tahbi at the same time. In this context, I would be very pleased if Pr. Hickman could spend a few weeks in Montpellier and I am sure that his stay here would be very profitable for all of us.

Yours sincerely

Fabien Gatti



GRUPE DE RECHERCHE EN ASTRONOMIE
ET ASTROPHYSIQUE DU LANGUEDOC

UMR 5024 – UMII/CNRS

INSTITUT
PHYSIQUE
MONTPELLIER

Montpellier, March 26, 2010
To Whom it May concern,

Invitation : for Pr. P. Hickman to the University of Montpellier II

My Institute GRAAL, of the university of Montpellier (UM2) is glad to support the scientific invitation of Pr. P. Hickman, from Dr. Fabien GATTI from the Institut Charles Gerhardt of the University of Montpellier. This visit is important since it will officially enlarge the collaboration between Pr. P. Hickman and myself, on the theoretical treatment of DR processes to Dr. F. GATTI, the specialist of a quantum mechanical wave packets method that is needed for the treatment of the dynamics of these processes. This visit will provide us the unique opportunity to sit the three of us around a table to decide how we can best combine our forces to successfully treat such processes.

During his stay, GRAAL will make sure that all laboratory facilities that Pr. Hickman might need will be provided to him.

Sincerely yours

Dr Dahbia Talbi
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PI of the Astrochemistry Group of GRAAL.
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