This proposal is representative of the projects currently on offer in our group. For more details of active research projects, please visit our webpage at: http://www.chem.leeds.ac.uk/People/Miranda.html

New theoretical methods for the analysis of molecular collision processes

Dr Marcelo Miranda

The purposes of this project are to develop genuinely new theoretical approaches for the description of molecular collisions, using mathematical techniques not yet employed for the study of this subject.

Our research group uses theoretical and computational methods to study the dynamics of molecular collisions, whether reactive or not. We try to explain how they proceed, what factors influence them, and when and how it is possible to exert control over a molecular collision and its outcome [1].

We are interested in the development of new theoretical approaches to this problem. In particular, we are interested in adapting new mathematical concepts and techniques (quantum geometry, quantum information theory, antieigenvalue analysis, and others) to the study of collision dynamics [2, 3]. This is a two-way avenue. On one hand, the new mathematical descriptions are bound to offer new perspectives and new insight into molecular collisions. On the other, molecular collisions have potential to work as excellent systems for the development through practical application of the new approaches.

This project will provide opportunities for the student to receive training in molecular quantum mechanics, new and advanced mathematics, and advanced scientific computer programming.

Please contact Dr. Marcelo Miranda (M.Miranda@leeds.ac.uk) for further details about this opportunity.

References

