1. Aim & motivation - Please explain the scientific and/or other motivation for the STSM and what scientific and/or other outcomes you aim to accomplish with the STSM.

The motivation for this short term scientific mission (STSM) stems from a PhD project being undertaken at University College London (UCL) to develop a computational method to calculate rate constants and cross sections for chemical reactions of interest to the plasma physics community. Ideally, this method should be non-system specific, computationally cheap, and relatively quick.

The method currently being explored at UCL involves the use of deMonNano, a density fuctional tight binding (DFT-B) code, part of a group of programs called deMon (density of Montreal), developed at the University of Montreal, Canada [see: http://demon-nano.ups-tlse.fr/]. The method is fast and on-the-fly, however is not yet durable and robust to give comparable results with literature values at plasma conditions. It is for this reason that a STSM to visit a deMonNano developer would be beneficial for the project. Dr Mathias Rapacioli, a co-developer of deMonNano, has agreed to host a visit to the Laboratoire de Chimie et Physique Quantiques (Université Paul Sabatier, Toulouse, France), in order to learn more about the code. The overall aim of the STSM is to visit Dr Rapacioli in Tolouse and spend a week learning how to integrate deMonNano into our process to calculate rate constants and cross sections for chemical reactions of interest to the plasma physics community.

As well as producing a reliable, fast, and on-the-fly computational method for calculating the rate constants and cross sections for chemical reactions, it is also hoped that the STSM will also enable a long-term relationship between UCL and Dr Rapacioli at Universite Paul Sabatier, which will enabling the computational method to be updated and supported as technology progresses in the coming years.

2. Proposed contribution to the scientific objectives of the Action.

This aim fits in with COST action CM1405, Molecules in Motion, as it aims to develop a novel way of simulating molecular reactions in a way that can yield reaction rates and cross sections in a cheap and computationally inexpensive manner.

3. Techniques - Please detail what techniques or equipment you may learn to use, if applicable.

The purpose of this STSM is to learn how to use and implement the deMonNano code for rate constant calculations. Currently, deMonNano is being used with success to calculate the rate constant and cross section at RTP, however when the pressure is reduced or the temperature is raised, results from calculations no longer accurately compare to experiment. It is hoped that visiting Dr Rapacioli and learning more about the implementation of deMonNano will solve these issues.

4. Planning - Please detail the steps you will take to achieve your proposed aim.

I will spend a week with Dr Rapacioli at the Universite Paul Sabatier, in order for him to teach and advise the best practices for using deMonNano. He will also be able to use his experience and expertise to see if there are any issues in our work so far. Hopefully, he will also be able to advise us on how to use deMonNano to describe molecular collisions involving halogens, as this feature is currently not readily available.