## Work plan

**Title**: Computational study of formation of triatomic molecules by radiative association

The project concerns theoretical calculations of radiative association rates. Radiative association means that two species come together and form a molecule by spontaneous emission of a photon. This is a very improbable process. Still, such rates are important for understanding the chemical evolution in interstellar space, particularly in dust poor regions. Experimental measurements of radiative association rates are extremely challenging due to their low probability of occurring and have only been successful for a very limited set of species. Also the theoretical calculations are most challenging.

Daria Burdakova is a first year PhD student in Gothenburg who will be performing calculations of radiative association. In Gothenburg there is extensive background experience in calculating radiative association rates for forming diatoms. We would now like to go on and attempt to calculate these rates also in the case of forming a chemically bound triatomic molecule. Professor Thierry Stoecklin at Bordeaux university is a world leading expert on this (see for instance T. Stoecklin, F. Lique and M. Hochlaf, Phys. Chem. Chem. Phys. 15:13818 (2013)) and the aim of this STSM is that Daria during the visit to Bordeaux learns so much that she can perform these type of calculations.

The plan is to start from a computer code that is available in Bordeaux and let Daria perform radiative association calculations for H2 + Na+ in a first study. It is expected that Daria during the visit in Bordeaux will learn to use and understand the structure of the computer code. Final calculations will thereafter be performed in Gothenburg and eventually a paper should result. We then expect this collaboration to go on and in a following joint study investigate CO + H-.