



14 August 2018

Dr. Sonja Grubisic
STSM coordinator
COST Action MOLIM

I am writing this letter to support Victoria Clark's application for a COST STSM at Laboratoire de Chimie et Physique Quantiques (Toulouse) to work with Dr Mathias Rapacioli. Victoria is a PhD student in my group working on molecular reaction rates for plasma applications. The aim of the project is development of robust computational protocols for quick estimates of reaction rates for small molecular systems exposed to high temperatures. One of the promising approaches is deMonNano, a DFT-B based molecular dynamics code. Dr Mathias Rapacioli is a co-developer of deMonNano, who's expertise would be most valuable for the project. The plan for the STSM in Toulouse is to build such a protocol based on deMonNano and to test it on a set of simple systems. Apart from the project itself, I also see this STSM as an opportunity for Victoria to expand her knowledge in electronic structure calculations, molecular dynamics and reaction rates calculations. It is also a great networking opportunity. The proposal therefore has my strong support.

Best wishes,

A handwritten signature in blue ink, appearing to read 'S. Yurchenko', written over the 'Best wishes,' text.

Sergey Yurchenko, Dr.
Reader in Physics
Physics and Astronomy, UCL