SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CM1405 - Molecules in motion (MOLIM)
STSM title: the theoretical treatment of the nuclear motion problem for aluminium bearing oxides compounds of astrophysical relevance.
STSM start and end date: 15/12/2018 to 15/03/2019
Grantee name: Mr Bilel Mehnen

PURPOSE OF THE STSM:

Within the framework of the collaboration between the Laboratoire de Spectroscopie Atomique Moléculaire et Applications (LSAMA), Université de Tunis El Manar, Tunisia and the Laboratoire de Modélisation Simulation Multi-Échelle (MSME), Université Paris-Est Marne-la-Vallée, France, supported by the COST Short Term Scientific Mission program, we carried out the theoretical treatment of the nuclear motion problem for aluminium bearing oxides compounds of astrophysical relevance using the accurate ab intio methods CCSD(T)/ aV(X+d)Z (x=T,Q and 5) and CCSD(T)-F12/VXZ-F12 Q) (x=D,T and Q).

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

We started by investigating the electronic structure of the low-energy states of the AlNX (X=O and S) molecules and its isomers. In these investigations, we obtained the full-dimensional ground-state potential energy surfaces of these species around their equilibrium geometries to determine the relative spectroscopic constants and deduce the rovibronic spectra.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

We characterized the electronic structure of the low-energy states of the AlNX (X=O and S) molecules and its isomers and we calculated the three-dimensional potential energy surfaces of the ground states of these molecules to be applied in variational treatments of the nuclear motion problem to deduce the rovibronic spectra.

FUTURE COLLABORATIONS (if applicable)

We plan to extend this study to the excited states of the AlNX (X=O and S) triatomic species.