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MOLIM Action CM1405

Dear MOLIM committee

I am writing to apply for Short Term Scientific Missions (*SSTM*) advertised on your website page. I was recently awarded a PhD in physical chemistry under the guidance of Professor Majdi Hochlaf from the University of Paris Est Marne-La-Vallée, France and Professor Nejm-Eddine Jaidane from the University of sciences of Tunis El Manar, Tunisia. Some parts of the PhD project were undertaken in the chemistry department at the University of Hull, UK under the supervision of Dr David Benoit.

My PhD project involved spectroscopic investigations of small molecules interacting with rare gas environments such as clusters, interfaces and matrices. This work focused on theoretical studies of the interactions between interfaces and the small molecules trapped in a matrix. The theoretical methods I have used include: the post Hartree Fock methods (e.g. MRCI, MP2, CC and CCSD(T)-F12) and the periodic density functional theory with the dispersion correction DFT-D3. These methods are used to describe the spectroscopic properties of CO in different environments and to describe the long range effects. The calculations were done using the Molpro, Gaussian and CP2K codes. Moreover, the interaction of imidazole electronic structure with gold surfaces $\text{Im}@Au(111)$ was studied using DFT-D3 approach.

So far, I had co-authored two papers in these subjects:

-K. Mahjoubi, D.M. Benoit, N.-E. Jaidane, M. Mogren Al-Mogren and M. Hochlaf, "Understanding of matrix embedding: a theoretical spectroscopic study of CO interacting with Ar clusters, surfaces and matrices", Physical Chemistry Chemical Physics 17 (2015)17159.

-S.Izzaouihda, K. Mahjoubi, H. Abbou El Makarim, N. Komaha and D.M. Benoit, "Adsorption of imidazole on Au(111) surface: Dispersion corrected density functional study", Applied Surface Science, 383 (2016) 233.

I am currently working on the vibrational spectrum of Van der Waals (VdW) systems. So I would like to have your scholarship to do: Clustering and embedded induced spectroscopies effects: Anharmonic spectra of small molecules interacting with rare gas environments (cluster, surfaces and matrices); the cases of H₂ and CO, neutral and charged diatomic. Studies from cluster to periodic approach. The main objective of my project is to do a computations of anharmonic spectra of embedded astrochemical molecules, from cluster approach to periodic calculations. (i) Cation and neutral of dihydrogen molecule interacting with rare gas clusters and trapped in matrix. (ii) Cation and neutral of carbon monoxide molecule interacting with rare gas clusters and trapped in matrix. Therefore, determination of equilibrium structures and the harmonic and anharmonic vibrational frequencies of these two small molecules interacting with different environments of rare gas; Cluster, surfaces and matrices.

In 2012, I was involved in the European Project 'CAPZEO' where the United Kingdom was part of it, which includes an international symposium, a summer training and two scientific research projects. The first project focuses on the electronic structure calculations for the CO₂ adsorption modelling on the Zeolitic Imidazolate Frameworks (ZIFs) at the atomic level. The second work deals with the theoretical study of CO₂ scattering on a liquid-gas interface at the microscopic level. The liquid side of the interface is modelled by a monolayer of ZIFs subunits adsorbed on a gold surface. During my previous research experience including the PhD and the current work, I acquired in-depth theoretical

knowledge of molecules and their interactions with different environments. Furthermore, my various professional experiences at the Spectroscopy Atomic Molecular and Applications Laboratory in Tunisia, the Modélisation et Simulation Multi-Échelle laboratory in France, the chemistry laboratory, University of Hull in the in the United Kingdom and the 'Laboratoire de Chimie Bio-organique et Macromolécule de Marrakech, University of Sciences of Marrakech' in Morocco equipped me with expertise in the abovementioned theoretical methods and calculation tools. My previous experience and skills helped me to succeed in different research directions, including two published journal papers and adapt in various working environments.

I look forward to profit your award to do my research subject at the chemistry department of the university of Hull, UK where I can bring my skills and broaden my knowledge to contribute with a high standard journal papers to your research work. Please do not hesitate to contact me if further information is required.

Yours sincerely,

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