Work plan

The work plan is to foster a collaboration between two groups, which are actively participating in the theme of the COST ACTION MOLIM. The group of ICTM, Institut for Chemistry, Technology and Metallurgy, at University of Belgrade and the group of MSME, MultiScale Modeling and Simulation, at University of Paris-EST Marne La Vallée.

Within this collaboration, the applicant will work at the Institut for Chemistry, Technology and Metallurgy, at Belgrade University .
During her visit within the MOLIM action, the Applicant, Rahma Dahmani, will be able to investigate the effect of a water molecule on the stability of Tz-Zn(II) complex with and without CO2 molecule by means of DFT and ab initio methods. This computational study could serve as a practical guide for understanding phenomena at molecular level which is very useful for the design of functionalized nanoporous materials, fluorescent polymer nanospheres and electrodes for CO_2 adsorption / separation / sequestration purposes or catalytic conversion of CO_2 in biological media.
In fact triazoles - metal clusters are highly recommended for the synthesis and design of diverse materials. These include new polynuclear metal complexes,[1] hybrid coordination polymers,[2] mixed metal metal-organic polyhedra networks, colloids, metal organic frameworks (MOFs),[3] highly porous (3,24)-connected framework NTU-105,[4] functionalized podand triazole-linked gold nanoparticles,[5] highly hydrophobic porous organic polymers [6] and 1D ring-like infinite chains polymers.[7]
From this theoretical study, Miss DAHMANI will be able to publish her results in peer-reviewed international journal such as JPCA or CHEMPHYSCHEM.

Miss DAHMANI will complete her work on Zn(II)-Tz complex with CO2 in the presence of H2O molecule as she has already finished the identification of equilibrium structures without the presence of water molecule by mapping the ground state potential energy surface (PES) of {Tz-Zn(II)}- CO_2 species to locate the potential coordinating sites between Tz-Zn(II) and CO_2 , where a systematic search of all possible positions of CO_2 around Tz-Zn(II) is carried out. These computations are done at the M05- 2X[8] functional with dispersion correction, Grimme's D3 [9], along with 6-311++G(d,p) basis set. The corresponding data will be used as starting point for the computations using other DFTs.

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