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Quantum and Monte-Carlo molecular dynamics investigations of the liquid anti-corrosive performance of a series of macrocyclic polyethers with a thiadiazolic core

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The corrosion inhibitive performance, in acidic medium, of a series of macrocyclic polyether compounds containing a thiadiazolic core: n-MCTH (n=1-5) which differ by the oxygen number in the macrocyclic polyether part, was studied on the basis of their degree of planarity, their global quantum electronic molecular descriptors and their local electronic proprieties (Fukui indices, Electrostatic molecular potential, Natural population atomic charges, Natural bond orbitals interaction) as well as their deformation capacity to adhere onto the metal surface, by using DFT calculations and Monte-Carlo system dynamics simulation. The proton affinity locating the most favorable site of protonation was evaluated and the competitiveness between neutral and protonated species in vacuo and in aqueous solution was also considered. The molecule 5-MCTH was found more reactive in vacuo and in aqueous phase. Moreover, the Fe-(N9N10)-like interaction involving 5-MCTH was found to be the strongest, in accordance with electrochemical and gravimetric results.

Speaker Biography

Aziz Aboulmouhajir has completed his PhD in Molecular Modeling and spectroscopy, at the age of 25 years from Instelling Antwerpen University in Belgium with High Distinction. He is holder of the STAS Prize of the Royal Academy of Sciences, Letters and Arts of Brussels, in Belgium. For the last ten years, he was head of the Molecular Modeling and Spectroscopy E2MS Team at Chouaib Doukkali University. He is currently professor and director of several thesis projects in Molecular Recognition and spectroscopy in Hassan II University (Morocco).

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