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2nd International Conference on

Materials Science and Materials Chemistry

March 20-21, 2019 | London, UK

Comparative quantum chemical and dynamic Monte Carlo investigations of the cytisine derivatives as green inhibitors for corrosion protection of carbon steel in HCl medium.

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The corrosion of metals and their alloys, which is harmful to the environment, limits industrial processes by efficiency as well as by cost. Green corrosion inhibitors are currently the most sought after, because of their availability, their lower cost, their biodegradability, the respect of health and environmental standards and, above all, their extremely high efficiency. This work focused on the theoretical study of the reactivity of the three major constitutive of alkaloids namely Cytisine, Dehydro cytisine and N-methyl cytisine - extracted from seeds of *Retama Monosperma (L.) Bois*s, a very abundant medicinal plant in the Abda-Doukkala region of Morocco - as green metal corrosion inhibitors [1-2], with the aim of rationalizing the relationship between their molecular structure and their inhibitory efficiency. In addition to the investigation of regioselectivity and competitiveness between neutral and protonated entities in aqueous media, global reactivity was quantified by a variety of molecular quantum descriptors, while local reactivity was followed by Fukui indices and molecular electrostatic potential. Both global and local reactivity show a notable competition between the three inhibitors, with a priority of Cytisine in both gas and aqueous phases. Moreover, in order to approach the interaction mechanics between molecule and metal surface and quantify the nature and the adsorption strength of the complex formed, we have used quantum mechanics as well as dynamics Monte Carlo simulation. All quantum calculations were done in B3LYP with the aug-cc-pvdz basis set and the C-PCM solvation model.

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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