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The theoretical investigation of reduction potentials and and spectroscopic properties of nitrobenzene and keto-enol molecules

This research focuses on gaining better insight into the experimental reductions potentials of some selected nitrobenze and keto-enol molecules using two slightly different free energy circles.

Some of the methods used include the high computational method of G3-(MP2)-RAD and low computational methods of different DFT functionals. The applied computational methods significantly reproduced the experimental reduction potentials to a very minimal error margin and also give better insight into the chemistry of the molecules. The chemistries of the molecules were described in terms of the change in their ionization energy, proton affinity, pKa, interaction energy of the fragments, hyperpolarizabilities, exaltation index, band gap, UV electron excitation and QTAIM properties. The results from the nitrobenze molecules indicate a very strong electron coupling between the fragment one (nitro group (NO2)) and three (para-substituent) via the benzene ring that constitute the fragment two.

The computed results of the β-keto-enol molecules clearly showed that the enol tautomers will easily undergoes reduction compare to the keto tautomers because of higher (less negative) reduction potential than their keto form.

Methodology
The CHPC installed Gaussian 09 and 16 were used for the computation. Other packages used are GAMES and BIO3D which were locally installed on the CHPC account. Some of the libraries used are OpenMPI and MPICH. In all of the computation works, the maximum core ever used was 10 with 24 processors in each.

Presenter Biography

Dr Adebayo Adeniyi is a both physical and inorganic chemist. He specializes on the application of quantum mechanics and molecular dynamics to study the properties of molecules amd give more scientific insight into the experimental spectroscopic analysis. He is NRF rated researcher as “Young promising researcher”. His research area covers the area of drug design, molecular electrochemistry, quantum and spectroscopic properties of small molecules and their applications.

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