1O02 Excited state reactivity index theory application on organic molecules

O Abhijit Chatterjee

アクセルリス株式会社

Abstract: This study aims to use the concept of ground-state reactivity index formalism within density functional theory (DFT) to predict the behavior of the excited state through the response function produced by weak electric field on chlorinated methane and chlorinated benzenes. A comparison was made between the geometry of ground state and the excited state for those moieties through configuration interaction (CI) method with Austin Model 1 Hamiltonian over the optimized geometry of DFT at the ground state. Results obtained through these two methodologies suggested that in terms of polarizability and heat of formation, DFT can reproduce the excited state qualitatively. Again, those results can be further validated through UV spectral data, generated using CI method. The reactivity index proposition at ground state shows the potential of DFT to simulate excitation.

Short discussion: The excited reactivity index is first proposed by Chattaraj et al [1]. We have taken the concept and aimed to look into the capability of DFT formalism to explore that excitation for small organic molecules.[2]

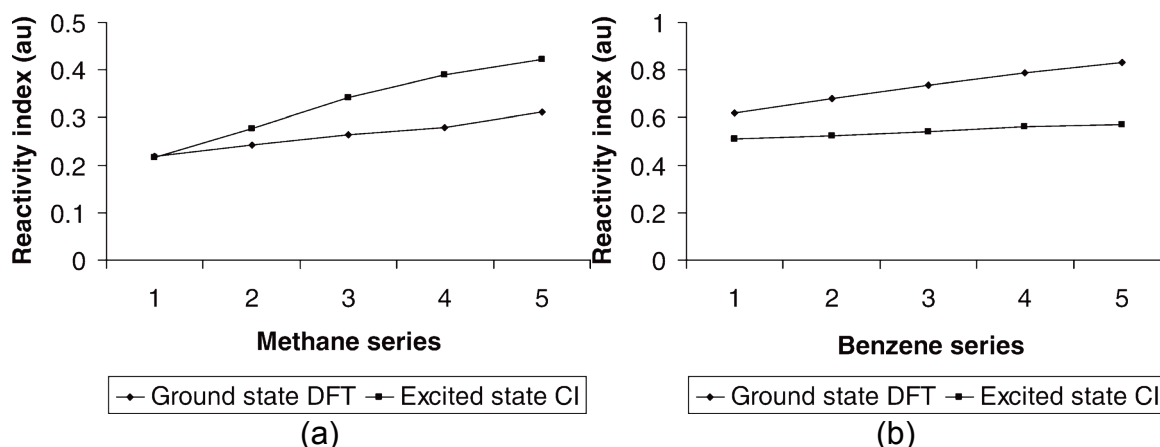(a)   (b)

Figure 1: The relative nucleophilicity as obtained for the (a) methane series and (b) benzene series with increase in the chlorine content for both the ground state and excited state.

One can conclude form this computational experiment that,the excited state properties can be similar to the ground-state properties over a series of CH_4, C_6H_6, and their chlorine-substituted compounds.

Reference:

1. Chattaraj, P. K.; Poddar, A. J. Phys. Chem. A   103,1274-1277 (1999)
2. Chatterjee A'; International J. of Quantum Chemistry, 111, 3821–3830(2011)