

Structures of Cation Doped Polyacenes and Its Binding Energies Across Polyacene Surface

Dr. Sharon Achamma Abraham

Assistant Professor, Department of Chemistry, Mar Thoma College, Tiruvalla-689103, India

ABSTRACT

The Binding energies of cation- π complexes are calculated computationally using the DFT method and the B3LYP functional. The binding energies in kcal/mol using B3LYP functional and 6-31+G (d,p) basis set in Gaussian09 has provided a source to design one-dimensional materials and to study the hopping of charges in one-dimensional materials. The Mulliken charges and ΔE in kcal/mol with bsse corrections are confirmed using B3LYP functional and 6-31+G (d,p) basis set in Gaussian09. Above benzene ring, a cation is located at a distance of 2.5 Angstrom units above the plane of the molecule and binding energy (ΔE) is calculated using B3LYP functional and 6-31+G (d,p) basis set, which shows difference between energy of benzene. Metal ion complex and sum of energy of benzene and cation M^+ . The binding energies of cation- π complexes on polyacenes are determined and study the hopping dynamics. Binding energies as well as hopping energies for the cations to polyaromatic hydrocarbons follow the order $Li^+ > Na^+ > K^+$. Binding energies (ΔE) decreases with size of the cation (M^+) and binding energy follows the order $Li^+ > Na^+ > K^+$. When binding energy (ΔE) decreases, incation- π complexes, reaction rate increases. This study has applications in computing rate of the reactions.

Keywords: Binding energy; functional; Transition State Structure; Potential Energy Surface; cation- π complex; polyacene

