Quantum Concepts and Natural Bond Orbitals in Chemistry: Applications of Computational Chemistry

Dr. Mohamed Ayoub, Department of Chemistry, University of Wisconsin-Washington County

In this work we demonstrate how essential quantum concepts to any real understanding of structure-reactivity relationship for diverse chemical systems of biological, and environmental interest. We employ density functional method (B3LYP) with 6-311++G** basis set and using natural bond orbital (NBO) methods along with natural resonance (NRT) to explore their bonding and nonbonding patterns which leads to best possible Lewis structure in their ground state.

We illustrate how quantum mechanics values of an overlap integral (S), stabilization energy ($\Delta E^{(2)}$) and interaction strength ($F_{i,j}$) can provide a complete understanding for the different chemical reactivity and possible resonance structures with their weights. In addition we provide 1d, 2d, and 3d plots for various NBOs of Lewis-type, non-Lewis type of bonding and nonbonding patterns and show their role in structure-reactivity relationship.