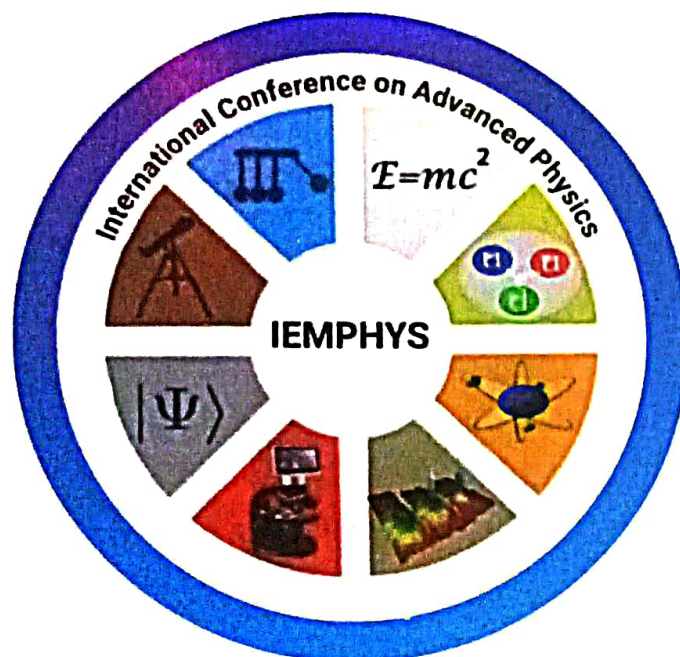


IEMPHYS-24

International Conference on Advanced Physics for
Sustainable Future: Innovations and Solutions



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Organised by

Department of Basic Science and Humanities,
Institute of Engineering & Management, Kolkata
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IEMPHYS-2024

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Exploring Electronic Properties and Molecular Reactivity of Aliphatic and Aromatic Hydrocarbons via DFT-Based Computations	86-87

Exploring Electronic Properties and Molecular Reactivity of Aliphatic and Aromatic Hydrocarbons via DFT based Computations

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This study aims to investigate the electronic properties of two distinct categories of hydrocarbons viz. (i) aliphatic type, and (ii) aromatic type, considering five different compounds such as ethane, ethene, ethyne (under aliphatic type), and benzene, toluene (under aromatic type) using Density Functional Theory (DFT). DFT calculations were performed using Gaussian 09W and GaussView 6.0 software. This study provides a detailed investigation of key electronic parameters, including the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), molecular electrostatic potential (MEP), density of states (DOS), and band structure for each compound. The objective is to gain insights into molecular reactivity, stability, and electron-donating/accepting abilities by examining these parameters. Analysis of the DOS provides information on available electronic states, while the band structure analysis reveals different energy levels and bandgaps, and offers insights into charge carrier mobility, and electronic transport. This comprehensive study not only enhances our understanding of the electronic characteristics and behaviors of aliphatic and aromatic compounds, but also lays a foundation for diverse applications, particularly in the realm of molecular science, materials science, and nanotechnology.

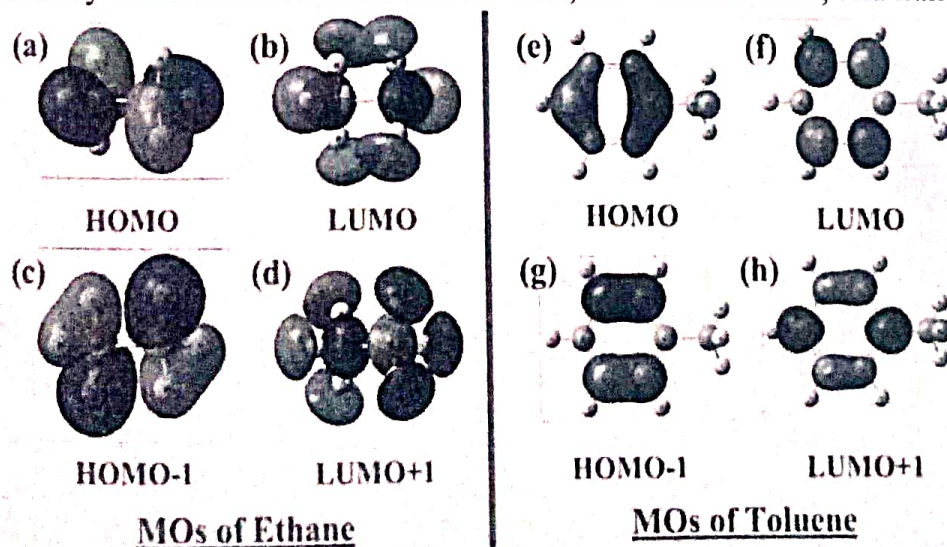


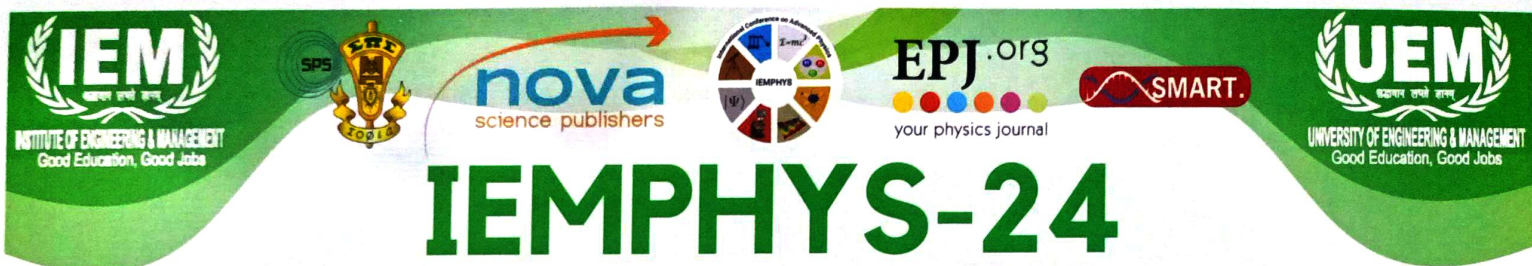
Fig. 1. Molecular Orbitals of (a-d) Ethane, and (e-h) Toluene

TABLE I. MOLECULAR ORBITAL ENERGIES OF ETHANE AND TOLUENE

Parameters	Ethane	Toluene
E_{HOMO} (eV)	-0.340	-0.236
E_{LUMO} (eV)	0.103	0.005
$E_{\text{HOMO-1}}$ (eV)	-0.340	-0.245
$E_{\text{LUMO+1}}$ (eV)	0.154	0.007
$E_{\text{HOMO-LUMO gap}}$ (eV)	-0.443	-0.241
$E_{[(\text{HOMO-1})-(\text{LUMO+1})]}$ gap (eV)	-0.494	-0.252

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