ENGINEERING CHEMISTRY

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Electronic Structure Determination – Example: Ethylene (C_2H_4)

- ✓ Ethylene (C_2H_4) is the simplest alkene with a C=C double bond.
- ✓ Electronic structure explains bonding, reactivity, and spectroscopy.
- ✓ Combines experimental (spectroscopy) and theoretical (MO theory, computation) approaches.

Hybridization and Bonding

- Each carbon atom is sp^2 hybridized.
- 3 sp^2 orbitals → 2 C–H σ bonds + 1 C–C σ bond.
- 1 unhybridized p orbital per C → forms π bond.
- Double bond (C=C) = 1 σ bond + 1 π bond.

Molecular Orbital (MO) Description

- σ system: strong localized framework bonds.
- π system: p-orbitals overlap to form π bonding and π* antibonding orbitals.
- HOMO = π orbital, LUMO = π* orbital.
- Basis for chemical reactivity of alkenes.

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Computational Determination

Steps:

1. Define geometry of C_2H_4.
2. Select Basis set (Mathematical functions).
3. Apply Method→ orbital energies & density.
4. Solve Equations → Get wave function/Electron Density
5. Visualize Electronic Structure → Orbital diagrams, density maps, HOMO and LUMO orbitals.

Application in Spectroscopy

- Photoelectron Spectroscopy (PES): measures σ and π orbital energies.
- UV–Vis: π → π* transition (~165–180 nm)
- IR: C=C stretch at ~1650 cm^{-1}
- NMR: Proton shifts

Applications

- Explains electrophilic addition reactions.
- Basis of alkene polymerization.
- Important in organic, catalytic, and photochemistry.
- Provides HOMO–LUMO insight for reactivity.

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THANK YOU

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