

**electronic  
Density Functional Theory**

**Cluster:**

- structure, energy, forces
- electrostatic moments
- harmonic frequencies
- charge transfer

**Small systems:**

- structure
- electrostatics in liquid phase
- fast dynamic processes

**Experiments**

- IR spectra
- X-ray/neutron scattering
- Dielectric spectra
- Thermodynamics, dynamics, and statics

**post-Hartree-Fock**

- continuum solvation models
- vibrational frequencies

**Molecular dynamics**