# Thesis Title: Bonding, Reactivity, and Properties of Many-Electron Systems: Conceptual-DFT and Information-Theoretic Approaches

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***Abstract-*** This thesis presents a comprehensive theoretical study of the bonding, reactivity, and properties of many-electron systems using Conceptual Density Functional Theory (CDFT) and Information-Theoretic Approaches (ITA). The unifying theme is that electron density and its derivatives, interpreted through CDFT and ITA descriptors, provide a transferable framework to understand chemical behavior across diverse systems. The systems investigated organic reactions, metal clusters, and QSPR models, represent different manifestations of the same principle: variations in electron density underpin reactivity, stability, and observable properties. Integrating these frameworks with complementary quantum-chemical tools establishes a unified density-based perspective bridging fundamental theory and chemical phenomena.

Molecular reactivity and bonding are governed by the interplay of electronic structure and external perturbations. While traditional orbital-based theories offer qualitative insights, CDFT provides quantitative reactivity measures through global and local descriptors derived from electron density, such as electronegativity, hardness, and electrophilicity. These connect quantum-chemical observables like ionization potential and electron affinity with intuitive chemical concepts. Complementarily, ITA quantifies electronic organization via measures such as Shannon entropy, GBP entropy, capturing molecular complexity and delocalization. Together, these frameworks enable consistent and quantitative interpretation of reactivity, selectivity, and stability.

In this thesis, CDFT and ITA descriptors were applied to elucidate unconventional selectivity patterns and predict favored reaction pathways, deepening the conceptual understanding of molecular reactivity. Extending to mechanochemical conditions, we examined how external forces modulate density, reactivity, and stability. Studies on Li, Na, and Li–Na alloy clusters revealed composition-dependent trends in bonding, delocalization, and entropy-driven stability.

Finally, the CDFT–ITA framework was employed in quantitative structure–property relationship (QSPR) modeling of 133 polychlorinated biphenyl congeners to predict physicochemical properties such as, n-octanol/water partition coefficient (log $K_{\mathrm{OW}}$) and enthalpy of vaporization ($\Delta_{\mathrm{vap}}H_{\mathrm{m}}$), achieving strong correlations with experimental data. The descriptors derived from the density serve as input variables for constructing QSPR models, allowing reliable statistical prediction of molecular and physicochemical properties. Thus, depending on context, the framework either computes electronic properties directly from first principles or predicts macroscopic properties statistically, both within a coherent density-based paradigm. Complementary analyses such as, energy decomposition analysis (EDA), quantum theory of atoms in molecules (QTAIM), Atom-Centered Density Matrix Propagation (ADMP), and nonlinear optical (NLO) property calculations reinforced the density-based interpretations.

Overall, this work establishes CDFT and ITA as a coherent, transferable foundation for understanding and predicting chemical behavior, linking microscopic electronic structure with macroscopic observables. It advances a unified, density-driven paradigm for modern theoretical chemistry.

## Keywords

Conceptual Density Functional Theory (CDFT), Information-Theoretic Approach (ITA), Reactivity Descriptors, Torquoselectivity, Mechanochemistry, Metal Clusters, QSPR Modeling