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QUANTUM-CHEMICAL MODELING OF THE ELECTRONIC STRUCTURE, REACTIVE SITES, AND CHEMICAL ACTIVITY OF A TKFV-BASED SORBENT–LIGAND

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Abstract:

Quantum-chemical modeling is an important approach for investigating the molecular structure, electronic properties, and chemical reactivity of functional sorbent–ligand systems. This article presents a theoretical framework for studying the electronic structure, reactive sites, and potential chemical activity of a TKFV-based sorbent–ligand. Particular attention is given to molecular geometry optimization, frontier molecular orbital analysis, electrostatic potential distribution, atomic charge estimation, and the identification of potential adsorption and coordination centers. Density functional theory (DFT) is considered a suitable computational approach for evaluating the relationship between molecular structure and chemical reactivity. The proposed methodology also includes the analysis of global reactivity descriptors, such as the HOMO–LUMO energy gap, chemical hardness, chemical potential, and electrophilicity index. These descriptors can help explain electron-donor and electron-acceptor properties and identify molecular regions potentially involved in interactions with target species. The study provides a methodological basis for predicting the adsorption behavior and coordination potential of the sorbent–ligand. Since the precise chemical structure and computational results for TKFV have not been provided, the discussion is presented as a research framework rather than as a report of completed numerical calculations.

Keywords: TKFV-based sorbent–ligand, quantum-chemical modeling, density functional theory, electronic structure, reactive sites, HOMO–LUMO energy gap, molecular electrostatic potential, adsorption, coordination chemistry, chemical reactivity.

Introduction

The development of efficient sorbent materials is an important direction in modern analytical, environmental, and coordination chemistry. Sorbents containing functional ligands can interact with target species through electrostatic attraction, hydrogen bonding, coordination interactions, and other intermolecular forces. The effectiveness of such materials depends on their chemical composition, molecular geometry, electronic structure, and the accessibility of their active centers.

Conventional experimental approaches provide essential information about adsorption capacity, selectivity, and stability. However, experimental measurements alone may not fully explain the molecular mechanisms responsible for the observed behavior. Quantum-chemical calculations complement experimental studies by providing information about electron distribution, molecular orbitals, charge localization, and the energetics of molecular interactions.

Density functional theory has become a widely used approach for examining the electronic structures and chemical reactivities of molecular systems. When applied appropriately, it can help identify possible coordination centers, compare alternative molecular configurations, and estimate the relative stability of complexes. Quantum-chemical approaches have also been used to investigate adsorption mechanisms and the interactions between functional groups and target metal ions [1–3].

The electronic properties of a sorbent–ligand determine, to a considerable extent, its ability to donate or accept electron density during chemical interactions. Atoms containing available lone pairs, negatively polarized functional groups, and regions with favorable electrostatic potentials may participate in adsorption or coordination. Nevertheless, the actual role of each center depends on the molecular environment, protonation state, solvent, target species, and geometry of the resulting complex.

In this context, quantum-chemical modeling of a TKFV-based sorbent–ligand can provide a theoretical basis for identifying its potentially reactive regions and evaluating the relationship between its electronic structure and chemical activity.

The aim of this study is to establish a quantum-chemical methodology for investigating the electronic structure, reactive centers, and potential chemical activity of a TKFV-based sorbent–ligand.

The specific objectives are:

To determine the optimized molecular geometry of the sorbent–ligand.

To investigate its frontier molecular orbitals and energy gap.

To analyze the molecular electrostatic potential and atomic charge distribution.

To identify potential adsorption and coordination centers.

To evaluate global chemical reactivity descriptors.

To formulate a computational strategy for examining interactions with selected target species.

2. Theoretical Background

2.1. Electronic structure and molecular geometry

The molecular geometry of a sorbent–ligand influences its stability, electronic distribution, and ability to interact with other chemical species. Bond lengths, bond angles, torsional angles, and intramolecular interactions determine the spatial arrangement of functional groups and the accessibility of potential reactive centers.

Geometry optimization is therefore an essential initial step in quantum-chemical modeling. It involves finding a molecular configuration corresponding to a stationary point on the potential energy surface. A subsequent vibrational-frequency calculation can help establish whether the optimized structure represents a local minimum. A structure with no imaginary vibrational frequencies is generally consistent with a local minimum within the selected computational model.

For a TKFV-based sorbent–ligand, geometry optimization should be performed after the chemical composition, connectivity, formal charge, and relevant protonation state have been established. If several conformations are possible, their relative energies should be compared to avoid relying on a single potentially unrepresentative structure.

2.2. Density functional theory

Density functional theory is based on the use of electron density to describe the electronic properties of a molecular system. Compared with many high-level wave-function methods, DFT can provide a practical balance between computational cost and accuracy for a broad range of molecular systems.

A general DFT calculation includes molecular structure preparation, selection of an exchange–correlation functional, specification of a basis set, geometry optimization, and analysis of the resulting electronic properties.

The computational level should be selected according to the chemical composition and intended application of the sorbent–ligand. For an organic ligand containing common light elements, a functional such as B3LYP or PBE0 combined with a suitable basis set may be considered as an initial approach. Dispersion-corrected methods may be necessary when noncovalent interactions contribute significantly to adsorption or complex formation

If the sorbent–ligand interacts with transition-metal ions, the calculation must account for the metal's electronic configuration, possible spin states, and suitable basis sets or effective core potentials where appropriate. Solvent effects should also be considered when the intended application involves aqueous solutions.

2.3. Frontier molecular orbitals

The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are important descriptors in qualitative molecular orbital analysis.

The HOMO represents the highest-energy occupied orbital, whereas the LUMO represents the lowest-energy unoccupied orbital. Their spatial distributions can indicate regions associated with electron-donor and electron-acceptor behavior.

A relatively small HOMO–LUMO gap is often associated with greater electronic polarizability or a potentially greater response to perturbation. However, the gap alone cannot establish the adsorption capacity, selectivity, or overall chemical activity of a sorbent. These properties also depend on molecular geometry, solvation, steric accessibility, interaction energies, and the structure of the target species.

Consequently, HOMO and LUMO distributions should be interpreted together with electrostatic potential maps, atomic charges, and calculated interaction energies.

2.4. Molecular electrostatic potential

Molecular electrostatic potential (MEP) analysis provides a spatial representation of the electrostatic environment surrounding a molecule. It can be used to identify regions that are relatively favorable for interactions with positively or negatively charged species.

Regions of negative electrostatic potential may be associated with electron-rich areas, while positive regions may be associated with electron-deficient parts of the molecule. These patterns can help identify candidate coordination sites and regions potentially involved in electrostatic interactions.

For a TKFV-based sorbent–ligand, MEP analysis should be used to examine the spatial distribution of electrostatic potential around its functional groups. The resulting map may indicate possible interaction regions, but the final assignment of reactive centers requires consideration of orbital localization, atomic charges, steric accessibility, and complexation energetics.

3. Materials and Methods

3.1. Construction of the molecular model

The first stage of the proposed computational workflow involves constructing the molecular structure of the TKFV-based sorbent–ligand using molecular modeling software. The structure must reflect the actual chemical composition and bonding pattern of the investigated compound.

Hydrogen atoms should be added according to the relevant protonation state. Formal charges, bond orders, and possible tautomeric forms should be checked before calculations are initiated. If the material consists of a ligand attached to a polymeric or inorganic support, an appropriate molecular fragment or representative cluster may be required. The selected model should retain the functional groups expected to participate in adsorption or coordination. At the same time, the limitations introduced by simplifying the full sorbent structure must be clearly acknowledged.

3.2. Geometry optimization and computational parameters

Geometry optimization may be carried out using a suitable DFT functional and basis set implemented in computational chemistry software such as Gaussian or ORCA. The precise method should be selected after the molecular composition and charge state have been confirmed.

The general computational workflow comprises:

preparation and verification of the initial molecular structure;
geometry optimization;
vibrational-frequency analysis;
calculation of frontier molecular orbitals;
mapping of molecular electrostatic potential;
evaluation of atomic charge distribution;
calculation of global reactivity descriptors;
modeling of interactions with selected target species.

For systems containing flexible functional groups, conformational sampling is recommended. Several plausible conformations should be optimized, and their relative energies should be compared. Where solvent molecules or charged species may substantially influence the electronic structure, solvent effects should be incorporated into the computational model.

3.3. Analysis of frontier orbital energies

The HOMO and LUMO energies should be extracted from the optimized molecular structure. Their spatial distributions should then be visualized to determine whether the frontier orbitals are localized on particular functional groups or distributed across the molecular framework.

The HOMO energy may provide a qualitative indication of electron-donor tendencies, while the LUMO energy may help characterize electron-acceptor tendencies. These interpretations are qualitative and should not be treated as direct experimental measurements of electron-transfer rates or adsorption efficiency.

The HOMO–LUMO energy gap should be calculated for the optimized structure and, where useful, compared across different conformers or chemical forms of the sorbent–ligand.

3.4. Global chemical reactivity descriptors

Global reactivity descriptors can provide an additional framework for interpreting electronic properties. Within a simplified frontier-orbital approximation, chemical hardness, chemical potential, and electrophilicity can be estimated using the HOMO and LUMO energies.

These expressions provide approximate descriptors under the chosen orbital-energy convention. More rigorous definitions may use vertical ionization energies and electron affinities obtained from separate calculations on the neutral, cationic, and anionic systems.

Chemical hardness describes resistance to changes in electron distribution within the adopted conceptual framework. The electrophilicity index provides an estimate of the energetic

tendency to accept electron density. Neither descriptor independently establishes the overall performance of a sorbent–ligand.

3.5. Identification of reactive sites

Potential reactive sites can be investigated by combining several complementary indicators
Atomic charge distribution: Partial charges may identify atoms with relatively electron-rich or electron-deficient character. Their values depend on the charge-partitioning method.
Molecular electrostatic potential: The electrostatic potential map can indicate regions potentially favorable for interactions with charged species.
Frontier molecular orbitals: HOMO and LUMO localization may help identify functional groups involved in donor–acceptor interactions.
Geometric accessibility: The spatial arrangement of functional groups determines whether a potential center can be approached by a target species.
Complexation energy: Calculations involving the sorbent–ligand and a target species can help evaluate the relative favorability of alternative binding configurations.
If the ligand contains suitable donor atoms, such as nitrogen, oxygen, or sulfur, these atoms may be examined as candidate coordination centers. Their actual participation must be established from the verified chemical structure and calculations rather than inferred from the presence of an element alone.

3.6. Modeling sorbent–target interactions

To investigate adsorption or coordination, a target species should be introduced into the computational model. Several plausible initial orientations and binding arrangements should be considered, followed by geometry optimization of each complex.
A useful quantity for comparing complex formation is the interaction or binding energy. One commonly used convention is:
With this convention, a negative value indicates that the optimized complex has a lower electronic energy than the isolated components at the corresponding computational level. The interpretation must account for the molecular charge states, reference structures, basis-set effects, and whether solvent or thermal corrections are included.
For reliable comparisons, all component calculations should use consistent computational settings. Basis-set superposition error may need to be considered, particularly for noncovalent complexes calculated with modest basis sets. Where the sorbent operates in solution, solvation free energies and relevant protonation equilibria may significantly influence the predicted interaction.

4. Results and Discussion: Expected Analytical Framework

4.1. Molecular geometry and structural stability

The optimized geometry is expected to provide the structural basis for examining the chemical behavior of the TKFV-based sorbent–ligand. The positions of its functional groups, local bond



geometries, and conformational flexibility can influence the accessibility of potential binding sites.

A frequency calculation should be used to verify whether the optimized configuration corresponds to a local minimum. If multiple conformations are identified, their relative energies should be examined before assigning a preferred molecular geometry.

Structural flexibility may have competing effects. It can facilitate adaptation to a target species, but it can also introduce a conformational energy penalty when the molecule adopts its bound configuration. Therefore, the lowest-energy isolated conformation does not necessarily correspond to the most favorable configuration for adsorption.

4.2. Electronic structure and frontier orbital distribution

Analysis of the frontier orbitals can help determine whether electron density is concentrated around functional groups potentially involved in adsorption or coordination. If the HOMO is localized near a suitable donor group, that region may be considered a candidate for electron donation. If the LUMO is concentrated in an electron-deficient region, it may indicate a potential pathway for accepting electron density.

These interpretations must remain conditional until the molecular structure and calculated orbital distributions are available. The HOMO–LUMO gap should not be used as the sole criterion for predicting chemical activity, because the orbital energies of an isolated ligand do not fully describe the energetics of a ligand–target interaction.

4.3. Electrostatic potential and potential binding centers

The electrostatic potential map can help distinguish molecular regions with different electrostatic characteristics. Negative-potential regions may attract positively charged species, while positive-potential regions may favor interactions with negatively charged species. Coordination to metal ions may also involve specific donor atoms whose lone-pair orbitals can interact with suitable metal orbitals.

The relative importance of these effects depends on the chemical environment. In aqueous systems, solvent molecules, ionic strength, and protonation equilibria may substantially alter the interaction pattern. Therefore, electrostatic potential maps should be interpreted alongside the optimized geometry and explicit or implicit solvent models where necessary.

4.4. Chemical reactivity and adsorption potential

The combination of frontier orbital analysis, electrostatic potential mapping, and global reactivity descriptors provides a multidimensional approach to investigating chemical reactivity. These descriptors can support comparisons between different structural forms of the ligand and help prioritize possible interaction sites for more detailed modeling.

Nevertheless, predicting sorption performance requires more than evaluating the isolated ligand. The adsorption capacity of a real material depends on the number and accessibility of binding sites, surface area, pore structure, diffusion, competing ions, solution pH, and

experimental conditions. Quantum-chemical calculations are most informative when integrated with experimental measurements and, where appropriate, molecular dynamics or adsorption-process modeling [2, 3].

4.5. Limitations and validation

The reliability of quantum-chemical predictions depends on the quality of the molecular model and the suitability of the selected computational method. Simplified molecular fragments may not reproduce the full electrostatic environment of a polymeric or inorganic support. In addition, approximate exchange–correlation functionals and basis sets can introduce uncertainties into calculated energies and charge distributions.

For these reasons, the final interpretation should include methodological limitations and, where possible, validation against spectroscopic, adsorption, or complexation data. Sensitivity to the choice of computational method should also be examined if the principal conclusions depend on small energy differences.

Because the molecular formula, structural representation, target species, and actual calculation outputs for TKFV have not been specified, no numerical orbital energies, atomic charges, binding energies, or adsorption efficiencies are reported here. These values should be included only after the corresponding calculations have been performed.

5. Scientific Significance and Practical Implications

The proposed modeling framework can contribute to the rational evaluation of TKFV-based sorbent–ligands by linking molecular structure with potential chemical reactivity. The combined analysis of geometry, frontier orbitals, electrostatic potential, and complexation energies can help narrow down candidate binding sites and guide subsequent experimental investigations

The practical value of the approach lies in its potential to reduce uncertainty during the initial stages of sorbent design. Instead of relying exclusively on trial-and-error experimentation, researchers can use molecular calculations to compare plausible binding configurations and identify structural modifications that may improve accessibility or interaction strength.

For environmental applications, the method could be extended to the selective binding of metal ions or other target species, provided that the chemical identity of the sorbent and the target is explicitly defined. Such applications require additional assessment of competing ions, pH dependence, regeneration, material stability, and performance under realistic operating conditions.

6. Conclusion

Quantum-chemical modeling provides a systematic approach to investigating the electronic structure, reactive sites, and potential chemical activity of a TKFV-based sorbent–ligand. The proposed methodology combines molecular geometry optimization, frontier molecular orbital

analysis, molecular electrostatic potential mapping, atomic charge estimation, and global reactivity descriptors.

The analysis of HOMO and LUMO distributions can help identify candidate electron-donor and electron-acceptor regions, while electrostatic potential maps and atomic charge distributions provide complementary information about possible interaction centers. Modeling of the ligand with selected target species can further clarify the relative favorability of alternative binding configurations.

However, the electronic properties of an isolated ligand cannot independently establish the adsorption capacity or selectivity of a complete sorbent material. Reliable conclusions require a chemically verified molecular structure, clearly specified computational parameters, analysis of relevant target species, and validation against experimental evidence.

The next stage of this research should therefore involve defining the exact TKFV chemical structure, conducting the proposed quantum-chemical calculations, reporting reproducible numerical results, and comparing the predictions with experimental adsorption or complexation data. Such an integrated approach can provide a stronger scientific basis for understanding and optimizing the performance of TKFV-based sorbent–ligands.

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