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Research paper

The Role of Quantum Chemistry in Complex Molecular Systems

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Abstract

Quantum chemistry provides a rigorous theoretical framework for describing molecular behavior at the electronic scale, offering capabilities that fundamentally surpass the explanatory and predictive limits of classical and semi-empirical models. Unlike classical approaches, which treat electrons implicitly or rely on parameterized interactions, quantum chemical methods explicitly resolve electronic structure, enabling reliable predictions of molecular geometries, reaction energetics, and electronic reactivity in chemically complex systems. This study critically examines the performance and limitations of quantum chemistry across four particularly challenging domains: transition-metal complexes, bond dissociation phenomena, near-degenerate electronic states, and magnetic or electronically excited systems. While Density Functional Theory (DFT) offers an efficient balance between accuracy and computational cost, its reliability can degrade in systems with strong electron correlation, necessitating the use of multi-reference and wave function-based methods. Through this comparative analysis, the study demonstrates how advances in quantum chemical theory and computation have significantly improved predictive accuracy, deepened understanding of chemical bonding and reactivity, and enabled practical progress in catalysis, spectroscopy, materials science, and photo-physics while also highlighting the methodological trade-offs that continue to define the field.

Keywords: *Density Functional Theory; Transition-Metal Chemistry; Multireference Methods; Bond Dissociation; Non-Adiabatic Phenomena; Magnetic Coupling; and Excited States.*

1. Introduction

Quantum chemistry, the application of quantum mechanics to chemical systems, lies at the heart of modern molecular science. It provides a rigorous framework for describing the behaviour of electrons within atoms and molecules, predicting properties such as bond energies, molecular geometries, and reaction pathways. Over the past few decades, the integration of theoretical principles with computational techniques has transformed chemistry from an observational science to a predictive one. Quantum chemistry applies the principles of quantum mechanics to understand, model, and predict the behaviour of atoms and molecules[1]. It is particularly powerful in studying systems where classical models fail such as transition metals, excited states, and bond-breaking processes. Quantum chemistry, the theoretical foundation that applies the laws of quantum mechanics to chemical systems, has transformed the way scientists understand molecular structure, bonding, and reactivity. Unlike classical chemical models, which rely on empirical observations, quantum chemistry describes matter at the subatomic level where the behaviour of electrons determines the chemical and physical properties of molecules. Through its mathematical framework, quantum chemistry provides a microscopic view of atomic interactions and enables the prediction of molecular properties with remarkable accuracy [2-3].

Over the past few decades, rapid advances in computational methods and computer power have extended the reach of quantum chemistry from simple diatomic molecules to complex systems containing transition metals, radicals, and large biomolecules. Theoretical approaches such as Hartree–Fock theory, post-Hartree–Fock methods, and Density Functional Theory (DFT) have become indispensable tools for chemists seeking to explore reaction mechanisms, electronic spectra, and energy landscapes [4]. These methods have allowed the simulation of chemical phenomena that are often inaccessible to direct experimental observation [5].

Particularly challenging are systems characterized by strong electron correlation and multiple interacting electronic states such as transition metal complexes, bond-breaking processes, molecules with near-degenerate electronic states, and magnetic or excited-state systems. In these cases, classical approximations fail to capture the subtleties of electronic rearrangements, spin couplings, and non-adiabatic effects. Quantum chemistry provides the only reliable approach to analyse and interpret these phenomena, offering both qualitative insights and quantitative predictions. Understanding the role of quantum chemistry in these complex molecular systems is essential not only for theoretical advancement but also for practical applications in catalysis, materials design, molecular electronics, and photo physics. The present study explores how quantum chemical principles and computational strategies contribute to the understanding of such systems, emphasizing their impact on both fundamental research and technological innovation [6].

Certain classes of systems such as transition metal complexes, reactive intermediates in bond-breaking processes, and species with near-degenerate or excited electronic states pose significant challenges for conventional chemical theories. Their behaviour is governed by intricate electronic interactions, correlation effects, and spin couplings that require quantum mechanical treatment. Understanding these

phenomena is crucial not only for advancing theoretical chemistry but also for practical innovations in catalysis, magnetic materials, and photochemical devices [7-8].
This paper discusses how quantum chemistry provides the conceptual and computational tools needed to study these complex systems, with emphasis on the specific roles it plays in (1) transition metal complexes, (2) bond-breaking processes, (3) molecules with near-degenerate electronic states, and (4) magnetic systems or excited states.

2. Methodology

This review synthesizes current theoretical, computational, and methodological advances that enable quantum-chemical investigation of complex molecular systems. The methodology integrates (i) a structured literature survey, (ii) comparative assessment of quantum-chemical formalisms, and (iii) analytical mapping of methods to the four targeted application domains: transition metal complexes, bond-breaking processes, near-degenerate electronic states, and magnetic or excited-state phenomena.

2.1. Literature survey and data collection

A comprehensive literature search was conducted using peer-reviewed journals (e.g., J. Chem. Theory Comput., J. Phys. Chem., Chem. Rev., Nature Chemistry), focusing on studies published in the last two decades. Seminal methodological papers were included to maintain historical continuity.

2.2. Categorization of quantum-chemical methods

Methods were grouped according to the dominant physical phenomena they are designed to capture:
1) Density Functional Theory (DFT): Widely used for ground-state energies, structures, and spin-state prediction in transition-metal systems.
2) Ab-Initio Correlated Methods: MP2, coupled-cluster (CCSD(T)), and perturbation-based approaches used to model reaction pathways and bond dissociation.
3) Multireference Approaches: Complete Active Space Self-Consistent Field (CASSCF), CASPT2, NEVPT2, and other multiconfigurational schemes employed for near-degenerate electronic states and strong correlation.
4) Excited-State Methods: Time-dependent DFT (TD-DFT), equation-of-motion coupled cluster (EOM-CC), and multireference configuration interaction (MRCI) applied to photochemical and spin-dependent processes.

Each method's advantages, limitations, computational scaling, and accuracy benchmarks were evaluated based on published validation studies [9].

2.3. Mapping computational methods to the four target areas

To ensure clarity and consistency, a structured matrix approach was used to link quantum-chemical tools to each of the four complex chemical scenarios:
1) Transition Metal Complexes: Methods were assessed in terms of their ability to treat electron correlation, ligand-field effects, spin–orbit coupling, and multiconfigurational character.
2) Bond-Breaking Processes: Techniques were evaluated for their capability to describe potential energy surfaces, barrier heights, reaction intermediates, and dynamical effects.
3) Near-Degenerate Electronic States: Focus was given to identifying methods robust against static correlation and orbital degeneracy.
4) Magnetic and Excited States: Approaches were reviewed based on their performance in predicting exchange coupling constants, spin densities, zero-field splitting, and excited-state energy landscapes.

2.4. Comparative assessment criteria

A consistent evaluation framework was applied across all quantum-chemical methods, emphasizing:
a) Accuracy and reliability: Agreement with high-precision experimental data or benchmark ab-initio results.
b) Computational cost: Scaling behaviour, basis-set requirements, and parallelization efficiency.
c) Transferability: Method robustness across chemical environments and electronic complexity.
d) Applicability to large systems: Feasibility in biomolecules, catalysts, materials, or extended clusters.

2.5. Integration of conceptual and computational insights

The final synthesis integrates quantum-mechanical principles—such as electron correlation, spin symmetry, non-adiabatic interactions, and potential energy surface topology—with computational performance trends reported in the literature. Cross-comparison allowed identification of the most effective methods for each chemical problem and highlighted emerging techniques relevant to future research (e.g., machine-learning-assisted quantum chemistry, localized correlation approaches, and quantum computing-integrated models) [10].

3. Results and Discussion

3.1. Quantum chemistry and transition metal complexes

Transition metal complexes are among the most electronically complex systems in chemistry due to partially filled d and f orbitals, which give rise to multiple oxidation states, variable coordination geometries, and diverse magnetic properties. Classical bonding models are often insufficient to describe these features, making quantum-chemical approaches essential. Density Functional Theory (DFT) is the most widely applied method for transition metal systems because it offers a practical compromise between accuracy and computational cost. DFT reliably predicts metal–ligand bonding, spin states, and optimized geometries, making it suitable for medium-to-large complexes. However, while DFT performs well for ground-state properties, its accuracy can depend strongly on the choice of exchange–correlation functional, particularly for systems with strong static correlation or near-degenerate spin states.

Quantum chemistry also provides a quantitative understanding of crystal field splitting, ligand field stabilization energy, and spin crossover behavior, which are central to interpreting magnetic and optical properties. In catalytic organometallic systems, such as those involved in olefin polymerization or hydrogenation, quantum-chemical simulations reveal reaction intermediates, activation barriers, and potential energy surfaces. Compared with semi-empirical approaches, ab initio and DFT-based calculations offer significantly improved predictive power, enabling rational catalyst design rather than post hoc interpretation. Thus, quantum chemistry functions both as a microscopic probe and a predictive framework linking electronic structure to experimentally observable chemical behavior (Table 1).

Table 1: Key Quantum-Chemical Insights into Transition Metal Complexes

Quantum-Chemical Concept	Application / Significance	Example System
Crystal Field Splitting (Δ)	Determines electronic configuration, colour, and magnetism	$[Fe(H_2O)_6]^{2+}$ vs $[Fe(CN)_6]^{4-}$
Ligand Field Stabilization Energy (LFSE)	Explains stability and preferred geometry	Octahedral vs Tetrahedral Co(II) complexes
Density Functional Theory (DFT)	Predicts electronic structure and spin states with reasonable accuracy	Fe(II) spin-crossover complexes
Potential Energy Surface (PES) Analysis	Reveals reaction mechanisms and activation barriers	Oxidative addition in Pd(II)/Pd(IV) catalysis
Orbital Interaction Analysis (Molecular Orbitals)	Explains metal–ligand bonding and reactivity	Ni(0)-olefin complexes in polymerization
Magnetic Moment Calculations (μeff)	Correlates with unpaired electron count	

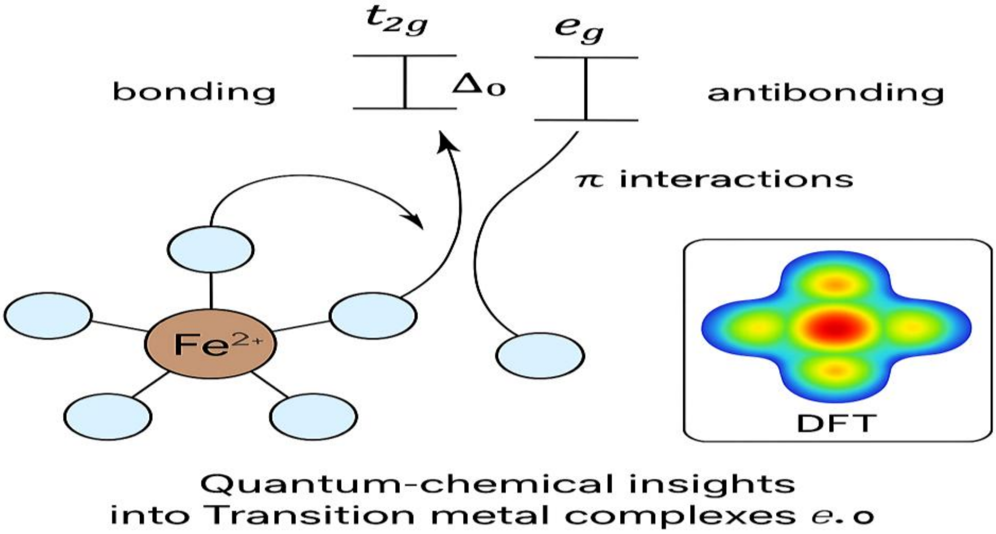

Fig. 1: Schematic Representation of Quantum-Chemical Features in a Transition Metal Complex.

3.1.1. Description (for diagram design)

- Centre atom: Transition metal (e.g., Fe^{2+})
- Six surrounding ligands arranged octahedrally (e.g., H_2O or NH_3)
- Include labelled d-orbital splitting diagram:
- $t_{2g}$and $e_g$levels with energy gap Δ_o
- Show metal–ligand σ and π interactions using arrows between orbitals
- Annotate regions representing bonding, antibonding, and nonbonding orbitals
- Optionally include a DFT computational output inset (e.g., electron density map or HOMO–LUMO visualization)

The Figure1, depicts an Fe^{2+} ion at the centre of an octahedral coordination sphere surrounded by six ligands. The d-orbital splitting diagram illustrates the energy difference (Δ_o) between the lower-energy $t_{2g}$and higher-energy $e_g$orbitals. Arrows indicate metal–ligand σ and π interactions, and the inset shows a DFT-calculated electron density map, highlighting regions of high electron probability. Thus, quantum chemistry serves as both a microscopic probe and a predictive tool, linking the electronic structure of transition metals to observable chemical and physical behaviour[12-13]

3.2. Quantum chemistry in bond-breaking processes

Bond-breaking and bond-forming reactions lie at the core of chemistry. These processes involve significant changes in electronic distribution, which classical mechanics cannot describe. Quantum chemistry provides a detailed view of potential energy surfaces (PES), allowing chemists to map the entire reaction pathway from reactants through transition states to products. Methods such as Hartree–Fock, post-Hartree–Fock (MP2, CCSD(T)), and DFT enable the calculation of bond dissociation energies, reaction barriers, and transition-state geometries. These calculations explain why certain bonds are easier to break, how energy is redistributed during reactions, and how substituents affect reaction kinetics.For example, in photochemical bond cleavage, quantum mechanical treatment reveals how electronic excitation alters the potential energy surface, lowering the energy barrier for bond dissociation [14-15]. Similarly, ab initio molecular dynamics simulations model how molecules evolve over time after absorbing energy as shown in Table 2.

Table 2: Chemical Insights intoBond-Breaking Processes

Quantum-Chemical Method	Primary Application	Key Outputs / Insights	Example Reaction System
Hartree–Fock (HF)	Approximate electronic structure	Qualitative PES and electron density	H_2 bond dissociation
MP2 (Møller–Plesset Perturbation Theory)	Correlation energy correction	Improved bond dissociation energy accuracy	$CH_4 \rightarrow CH_3 + H$
CCSD(T)	High-accuracy benchmark method	Precise activation energies, transition states	SN2 or hydrogen transfer reactions
Density Functional Theory (DFT)	Balance of cost and accuracy for large systems	Activation barriers, optimized geometries	Catalytic hydrogenation
Ab initio Molecular Dynamics (AIMD)	Time-resolved bond dynamics	Real-time visualization of bond formation/breaking	Photoexcited N_2O dissociation
Time-Dependent DFT (TD-DFT)	Electronic excitation and photochemistry	Excited-state PES mapping	Photochemical bond cleavage in NO_2

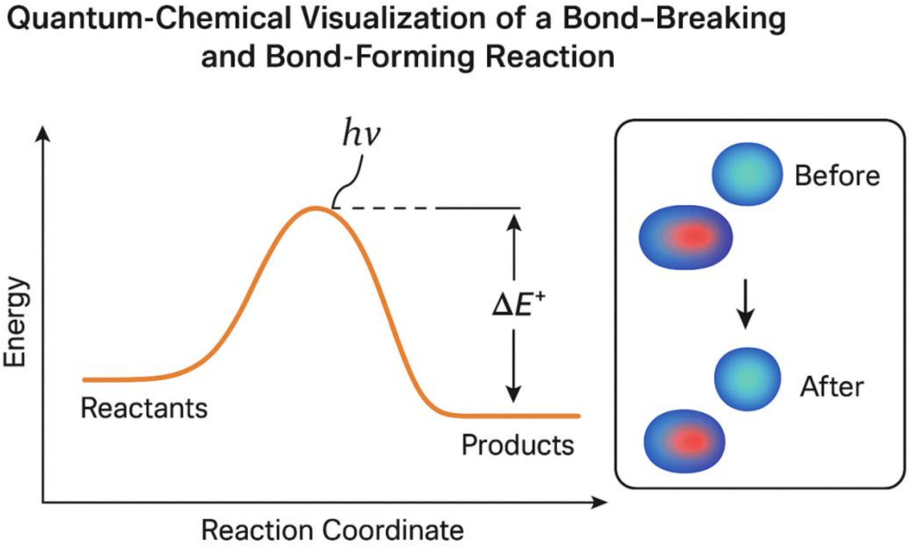

Fig. 2: Quantum- Chemical Vid-Bod-Breaking Aso.

3.2.1. Description (for diagram design)

1) A potential energy surface (PES) diagram showing the energy profile along the reaction coordinate:
2) Reactants → Transition State → Products
3) Label energy barrier ($\Delta E^{\ddagger}$) and bond dissociation energy (BDE).
4) Include a side panel inset showing: 1. Electronic density maps or orbital overlap changes before and after bond cleavage.2. Indication of HOMO–LUMO interactions during bond formation.
5) Optionally include a photon (hv) arrow to represent photochemical excitation.

Figure 2,shows that Quantum chemistry thus provides a quantitative and visual understanding of chemical reactivity, helping to predict reaction outcomes, optimize reaction conditions, and design molecules with tailored bond strengths [16].

3.3. Molecules with near-degenerate electronic states

Some molecules, such as diradicals, conjugated systems, and transition-state species, exhibit near-degenerate electronic configurations—states where multiple electronic structures have similar energies. In such systems, electron correlation effects are strong, and a single-reference method (like Hartree–Fock or standard DFT) becomes inadequate. To accurately describe these systems, multi-configurational methods such as CASSCF (Complete Active Space Self-Consistent Field) and MRCI (Multi-Reference Configuration Interaction) are employed [17-20]. These approaches consider multiple electronic configurations simultaneously, capturing both static and dynamic electron correlation.

Quantum chemistry enables the study of conical intersections, points where potential energy surfaces of different electronic states intersect. These intersections are critical in non-adiabatic processes such as internal conversion and photoisomerization, where electronic and nuclear motions are strongly coupled. Such analyses are indispensable for understanding the mechanisms of photochemical reactions, energy transfer, and spin-state transitions. For instance, the photo physics of retinal (in vision) and the functioning of photovoltaic materials depend on near-degenerate state dynamics that can only be captured by quantum mechanical models[18-19]. Near-degenerate electronic configurations states where multiple electronic structures have similar energies represent some of the most challenging systems in computational chemistry. In such systems, electron correlation effects are strong, and a single-reference method (like Hartree–Fock or standard DFT) becomes inadequate. To accurately describe these systems, multi-configurational methods such as CASSCF (Complete Active Space Self-Consistent Field) and MRCI (Multi-Reference Configuration Interaction) are employed [20].' These approaches consider multiple electronic configurations simultaneously, capturing both static and dynamic electron correlation. Quantum chemistry also enables the study of conical intersections, points where potential energy surfaces (PES) of different electronic states intersect as shown in Table 3.

Table.3: Key Quantum-Chemical Insights into Molecules with Near-Degenerate Electronic States

Method	Type	Main Advantage	Limitation	Typical Applications
Hartree–Fock (HF)	Single reference	Simple and fast	Fails for near-degeneracy	Ground-state calculations
DFT (Density Functional Theory)	Single reference	Cost-effective for large systems	Poor for multi-reference states	Transition-metal chemistry
CASSCF (Complete Active Space SCF)	Multi-reference	Captures static correlation accurately	High computational cost	Conical intersections, excited states
MRCI (multi-Reference CI)	Multi-reference	High accuracy (includes dynamic correlation)	Computationally expensive	Photochemical reactions
CASPT2 (CASSCF + Perturbation Theory)	Multi-reference hybrid	Balances cost and accuracy	Sensitive to active space selection	Organic photochemistry, spin-crossover
Non-Adiabatic Molecular Dynamics (NAMD)	Multi-surface dynamics	Models' energy flow between surfaces	Requires PES coupling data	Photoisomerization, internal conversion

3.3.1. Conical intersection and near-degenerate electronic states

- Two potential energy surfaces (PES) plotted along a reaction coordinate: Ground state (S_0) and excited state (S_1) intersecting at a conical intersection point (CI).
- Include arrows showing non-radiative transition (internal conversion) from $S_1 \rightarrow S_0$.
- Energy (vertical axis) vs nuclear coordinate (horizontal axis).
- On the right, include a small inset showing overlapping electronic orbitals before and after excitation.
- Optional labels: Excitation (hv), Relaxation, Conical Intersection (CI) as shown in Figure 3.

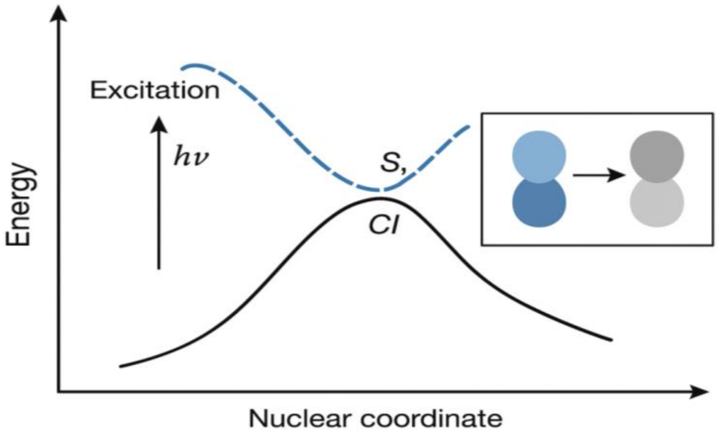

Fig. 3: Conical Intersection and Near-Degenerate Electronic States.

These intersections are critical in non-adiabatic processes such as internal conversion and photoisomerization, where electronic and nuclear motions are strongly coupled. Such analyses are indispensable for understanding the mechanisms of photochemical reactions, energy transfer, and spin-state transitions. For instance, the photo physics of retinal (in vision) and the functioning of photovoltaic materials depend on near-degenerate state dynamics that can only be captured by quantum mechanical models [21-23].

3.4. Magnetic systems and excited states

Magnetic and excited-state systems represent another frontier where quantum chemistry plays a defining role. The magnetic properties of molecules arise from unpaired electron spins and their couplings, which are quantum in nature. Quantum chemical calculations can determine exchange coupling constants, spin densities, and magnetic anisotropies, providing insight into the origin of magnetism in coordination compounds and molecular magnets. In excited-state chemistry, the absorption of light promotes electrons from occupied to unoccupied molecular orbitals, creating new electronic configurations. These states govern fluorescence, phosphorescence, and photochemical reactivity. Methods like Time-Dependent DFT (TD-DFT) and Configuration Interaction Singles (CIS) are used to predict absorption spectra, excitation energies, and transition dipole moments. Quantum chemical approaches have elucidated the excited-state behaviour of luminescent metal complexes, organic dyes, and semiconductor clusters [24]. They also enable the rational design of materials for OLEDs, solar cells, and photocatalysts by revealing how structural modifications influence electronic transitions. Thus, quantum chemistry bridges the gap between electronic structure and measurable magnetic or photo physical phenomena as shown in Table 4.

Table. 4: Chemical Insights into Magnetic Systems and Excited States

Property / Process	Quantum-Chemical Method	Key Outputs / Parameters	Typical Applications
Exchange coupling (J)	Broken-symmetry DFT, CASSCF	Magnetic exchange constant, spin coupling	Molecular magnets, transition-metal dimers
Spin density distribution	DFT, EPR parameter calculation	Localization of unpaired electrons	Radical species, metalloproteins
Magnetic anisotropy (D, E)	Spin–orbit coupling via DFT or ab initio	Zero-field splitting parameters	Single-molecule magnets
Excited-state energies	TD-DFT, CIS, CASSCF	Vertical and adiabatic excitation energies	UV–Vis absorption spectra
Fluorescence / phosphorescence lifetimes	Spin–orbit coupled TD-DFT or SOC-CI	Radiative and non-radiative decay rates	Luminescent metal complexes
Photochemical pathways	Surface-hopping dynamics, CASPT2	Potential energy surfaces of excited states	Photocatalysis, energy transfer in solar cells

3.4.1. Quantum-chemical representation of magnetic and excited-state phenomena

- Left side

Depict a transition metal complex(e.g., Mn_2 or Fe (III) showing two magnetic centres with arrows representing spin alignment (parallel / antiparallel).Label exchange coupling (J) and spin density (ρs) contours.

- Right side: Include a Jablonski diagram showing
- Ground state (S_0), singlet excited state (S_1), and triplet state (T_1).
- Upward arrow labelled Absorption (hν).
- Downward arrows showing Fluorescence ($S_1 \rightarrow S_0$) and Phosphorescence ($T_1 \rightarrow S_0$).
- The combined figure visually connects magnetic interactions with excited-state photo physics, representing how quantum chemistry models both.

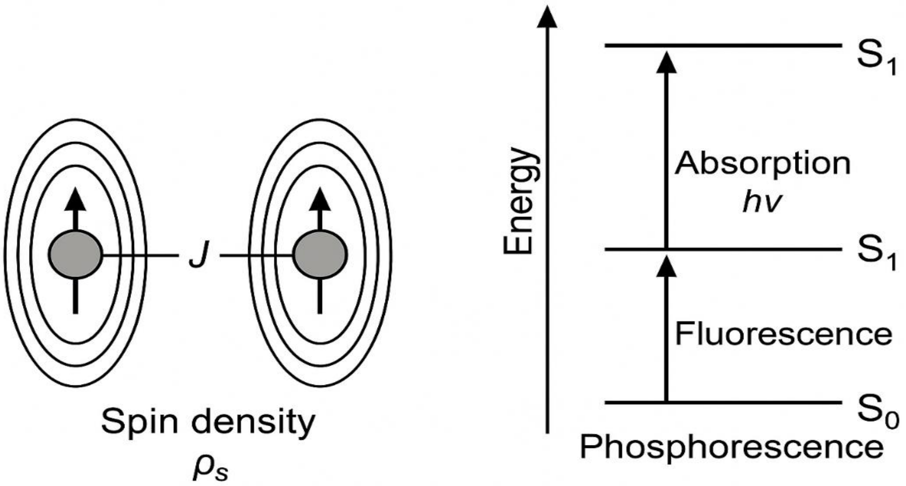

Fig. 4: Quantum-Chemical Representation of Magnetic and Excited-State Phenomena.

Magnetic and excited-state phenomena represent frontier areas where quantum chemistry provides indispensable insight into molecular behaviour beyond the ground state. Magnetic properties arise from unpaired electron spins and their couplings, which are inherently quantum in nature. Quantum chemical calculations enable the determination of exchange coupling constants, spin densities, and magnetic anisotropies, offering detailed understanding of magnetic interactions in transition metal complexes, molecular magnets, and radical species. Excited-state systems, on the other hand, involve electron transitions between molecular orbitals that govern photophysical and photochemical processes. Methods such as Time-Dependent Density Functional Theory (TD-DFT) and Configuration Interaction (CI) allow prediction of excitation energies, oscillator strengths, and electronic transition probabilities. These calculations are critical for interpreting absorption spectra, luminescence, andphotoinduced charge-transfer dynamics as shown in Figure 4. By integrating magnetic and excited-state modelling, quantum chemistry provides a unified framework for exploring spin-dependent reactivity, energy transfer mechanisms, and design of optoelectronic or photo functional materials, thus bridging fundamental theory with technological applications [25-26].

Table 5: Overview of Quantum Chemical Methods and Their Applications

Area	Quantum Chemistry Role	Key Methods	Applications
Transition Metal Complexes	Electronic structure, bonding, spin states	DFT, Ligand Field Theory	Catalysis, spectroscopy
Bond-Breaking Processes	Reaction paths, activation energies	Ab initio, CCSD(T)	Reaction kinetics, photochemistry
Near-Degenerate States	Multiconfigurational effects	CASSCF, MCSCF	Photochemical reactions, diradicals
Magnetic/Excited States	Spin coupling, electronic transitions	TD-DFT, CI	Magnetism, spectroscopy, luminescence

Table 5 provides an overview of major quantum chemical methods and their applications across four challenging molecular domains. In transition metal complexes, quantum chemistry plays a central role in elucidating electronic structures, metal–ligand bonding, and spin-state energetics. Methods such as Density Functional Theory (DFT) and Ligand Field Theory are widely employed to model catalytic activity and interpret spectroscopic properties. For bond-breaking processes, quantum chemical calculations reveal detailed reaction pathways and activation energies. High-level ab initio and coupled cluster [CCSD(T)] methods enable accurate characterization of transition states, which is critical for understanding reaction kinetics and photochemical mechanisms [27-28].

In systems with near-degenerate electronic states, where multiple configurations contribute significantly to the wavefunction, multiconfigurational approaches such as CASSCF and MCSCF are essential [29]. These techniques capture strong correlation effects and are vital for studying diradicals, excited-state crossings, and photochemical reactions [30]. Finally, in magnetic and excited-state systems, quantum chemistry provides insight into spin coupling, electronic transitions, and magneto-optical behaviour. Methods such as Time-Dependent DFT (TD-DFT) and Configuration Interaction (CI) are commonly used to describe magnetism, luminescence, and spectroscopic properties of molecular materials [31-32]. Overall, these approaches demonstrate how modern quantum chemical tools enable precise modelling of complex molecular phenomena, bridging theory and experiment across diverse areas of chemistry and materials science [33]. Thus, quantum chemistry bridges the gap between electronic structure and measurable magnetic or photophysical phenomena. The four domains discussed transition metal complexes, bond-breaking, near-degenerate states, and magnetic/excited systemsshare a common challenge: all involve complex electronic correlations beyond the scope of classical or semi-empirical models. Quantum chemistry provides the theoretical and computational machinery to decode these complexities [34]

Recent developments, such as machine-learning-assisted quantum chemistry, quantum computing algorithms for electronic structure, and hybrid quantum classical methods, promise even greater accuracy and scalability. These innovations could revolutionize how chemists simulate large and electronically intricate systems in real time. Moreover, the integration of quantum chemistry with spectroscopic data and molecular dynamics simulations allows direct comparison with experimental observations, validating theoretical models and guiding new experiments [35].

4. Conclusion

Quantum chemistry has evolved into a cornerstone of modern molecular science, enabling the understanding and prediction of complex chemical behaviour at the electronic level. In transition metal complexes, it explains bonding and reactivity; in bond-breaking processes, it maps reaction mechanisms; in near-degenerate systems, it captures multi-configurational electronic structures; and in magnetic or excited states, it predicts spin and photo physical phenomena. By combining rigorous quantum theory with computational innovation, quantum chemistry continues to bridge fundamental understanding and technological application informing the design of catalysts, materials, and molecular devices that shape the future of chemistry and materials science.

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Authors' Contributions

The author has contributed to data analysis, drafting, and revising of the article and agreed to be responsible for all aspects of this work.

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