Radical Helicene project literature review

Joseph Harries (02034665)

Historical background and theoretical overview:

In organic chemistry, the discovery and early development of helicenes represented a critical turning point. The unique helical structures that result from ortho-fused benzene rings define helicenes. These chiral compounds have attracted a great deal of scientific attention ever since Newman and Lednicer synthesised [6]helicene in 1955. Because of their chirality, helicenes are optically active and useful in a variety of applications, including stereochemistry and chiral recognition. This is due to their helical structure. Early studies concentrated on creating various helicene derivatives and investigating their basic characteristics. The potential of helicenes' distinctive optical properties, such as optical rotation and circular dichroism, in chiral light-matter interactions has been thoroughly investigated. Since then, improvements in synthetic techniques have made it possible to create increasingly intricate helicene structures with tailored properties for specialised applications.

The electrical characteristics and stability of stable neutral radicals, including trityl and phenalenyl radicals, are exceptional because of the steric protection provided by bulky substituents and the delocalization of the unpaired electron. These radicals have been studied since the middle of the 20th century and have demonstrated a lot of promise for electrical uses. The goal of incorporating stable radicals into organic semiconductors is to improve stability and charge transport capabilities. Studies have shown that conjugated systems with radicals such as triarylmethyl and phenalenyl have much better charge carrier mobility and overall material performance (Ravat et al., 2020).

The field of spintronics uses the electron's inherent spin and electrical charge to create electronic devices. In contrast to conventional electronics, which only considers an electron's charge, spintronics looks to the spin degree of freedom to provide additional functions and enhance device performance. Spin is the inherent angular momentum of electrons that may be orientated "up" or "down," creating magnetic moments. A substance becomes magnetised when a significant number of electron spins align in it, producing a magnetic field. A quantum mechanical magnetoresistance effect known as giant magnetoresistance (GMR) is seen in thin films made up of alternating ferromagnetic and non-magnetic layers. GMR, which was discovered in the late 1980s, revolutionised read-head and magnetic storage technology. These materials are valuable in hard drive read heads because they greatly alter in resistance when exposed to an external magnetic field. A thin layer of non-magnetic material sits between two ferromagnetic layers to form spin valves. The resistance varies as a function of the magnetic moments' relative alignment inside the ferromagnetic layers. A thin insulating layer sits in between two ferromagnetic layers in magnetic tunnel junctions, or MTJs. The resistance changes according to the ferromagnetic layers' spin alignment when electrons tunnel through the insulator.

The CISS effect occurs when electrons with a particular spin orientation are preferentially transmitted by chiral compounds. This phenomenon provides a technique to create and modify spin-polarized currents without ferromagnetic materials, which has important implications for spintronics. Chiral molecules, like helicenes, are non-superimposable on their mirror counterparts and exist as enantiomers. One spin state may be transmitted preferentially over another when electrons go through a chiral molecule due to the interaction between the electron spin and the chiral potential, Spin-orbit coupling (SOC), in which an electron's velocity is associated with its spin. SOC effects can cause transmitted electrons in chiral compounds to become spin polarised, explaining the observed CISS effect.

π-conjugated systems, consisting of alternating single and double bonds that permit delocalized π-electrons, are the building blocks of organic semiconductors. The delocalization is essential to the material's electrical conductivity. The energy gap between the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO) governs these materials' electronic characteristics. Electron transfers and band transport are two types of charge transport mechanisms found in organic semiconductors. Charge carriers in disordered organic materials migrate by hopping between localised states; this process is dependent on molecular connections and organisation as well as temperature activation. Similar to band conduction in inorganic semiconductors, charge carriers in highly organised crystalline organic materials can flow through delocalized states, leading to better mobility than electron transfer reactions.

A framework for comprehending electron transfer reactions, which are essential to charge transport in organic semiconductors, is provided by Marcus Theory. The energy needed to rearrange the surrounding environment and molecular structure during an electron transfer event is known as the reorganisation energy. It comprises reorganisation energies that are external (solvent or lattice) as well as internal (intramolecular). Marcus Theory states that the driving force (ΔG0) of the reaction and the reorganisation energy have an impact on the rate of electron transfer. For the electron transfer, the activation energy (G\*) is provided by:

G∗ = (λ+ΔG0)2/4λ

This equation shows that the electron transfer rate increases as the reorganization energy decreases and the driving force is optimized. The rate constant for electron transfer can be expressed as:

kET = νNe−G/kT

where kB​ is the Boltzmann constant, T is the temperature, and ν is a frequency factor related to molecular vibrations.

### Stabilised neutral radicals and helicenes have a lot of potential for use in organic electronics and spintronics. The CISS effect in helicenes makes it possible to design spin filters and other spin-polarized current-dependent devices in spintronics. Higher spin coherence and better charge transport can be attained by organic semiconductors that incorporate these materials, which makes them perfect for cutting-edge electronic devices like organic light-emitting diodes (OLEDs), organic photovoltaics (OPVs), and organic field-effect transistors (OFETs). These materials have the potential to be used in quantum computing and molecular electronics. By controlling electron spin and charge transport at the molecular level, these materials can be used to create electronic devices that are more flexible, scalable, and efficient, highlighting the research field's relevance in a wider context.

Literature review:

### General reading on Helicenes and Helicene radicals in research:

### "Helicenes—A New Class of Organic Spin Filter"

This work is a general paper that discusses important developments in our knowledge of the helicenes' chirality-induced spin selectivity (CISS) effect. Helicenes have a strong CISS effect because of their helical structure, which allows them to interact preferentially with electrons of a particular spin and produce spin-polarized currents. This phenomenon is especially interesting because helicenes act as organic spin filters because their chirality determines the spin orientation of the electrons that flow through them. The researchers point out that even though helicenes are made up of light elements, which generally have weaker spin-orbit coupling than heavy elements, the CISS effect in helicenes can achieve significant spin polarisation, even exceeding that seen in conventional ferromagnetic materials.

### Helicene-based devices were used in this study's experimental validation to measure magnetoresistance. The experiments confirmed that helicenes are capable of spin-filtering by showing antisymmetric magnetoresistance versus magnetic field plots. Based on these results, it appears that helicenes can be used in spintronic devices without ferromagnetic components. Additionally, the study offers thorough understandings of the molecular processes behind the CISS effect, backed by both experimental and theoretical data.

### "Helicene Radicals: Molecules Bearing a Combination of Helical Chirality and Unpaired Electron Spin"

The synthesis, structure, and characteristics of helicene radicals—which peculiarly combine unpaired electron spins and helical chirality—are examined in this summary paper. Redox reactions that introduce unpaired electrons into helical π-conjugated systems yield helicene radicals. The study describes in detail how these radicals are stabilised. By using bulky substituents to shield the radical centre and delocalizing the unpaired electron over the helical framework, the stabilisation is accomplished.

The main conclusions of this study highlight how the helical structure of helicene radicals increases their stability. For practical applications in electronic devices, this stability is essential. The unpaired electron is delocalized, which contributes to the stability and electronic properties of the radical, according to a detailed electronic structure analysis performed with Density Functional Theory (DFT) and Electron Paramagnetic Resonance (EPR) spectroscopy (Murafuji et al., 2020; Tani et al., 2020). Using methods like electron paramagnetic resonance (EPR) and electron nuclear double resonance (ENDOR), the study delves deeper into the magnetic characteristics of helicene radicals. By revealing details about the interaction between nuclear and electron spins, these methods shed light on the spin distribution and hyperfine coupling constants in radical molecules (Ravat et al., 2020). Zeeman splitting is examined in the study along with its consequences for themagnetic behavior of helicene radicals under an applied magnetic field.

Detailed structural information about helicene radicals was obtained through X-ray diffraction studies, which demonstrated the impact of π-stacking and steric interactions on the molecular geometry and electronic properties (Ravat et al., 2020). The extensive information on bond lengths and torsional angles provides insights into the structural elements stabilising the radical species. For those interested in investigating helicene radical applications in spintronics, in particular, this paper provides a critical framework for future research on the subject. An excellent basis for comprehending how these molecules can be optimised for use in cutting-edge electronic devices is provided by the thorough examination of their structural, magnetic, and electronic characteristics.

This work provides a methodological framework for the synthesis and characterization of helicene radicals for future investigations. To design spin-coherent organic semiconductors, similar approaches can help explore the interaction between helical chirality and unpaired electron spin. This paper's demonstration of the integration of experimental methods and computational modelling offers a well-defined framework within which my research will operate. The theory and comprehension of the particular class of molecules surrounding my project, as well as important details on previously synthesised radical helicenes that might be worth looking into, will be greatly aided by this paper.

“A Computational Exploration of the Crystal Energy and Charge-Carrier Mobility Landscapes of the Chiral [6]Helicene Molecule”

Rice et al. performed a comprehensive computational analysis to investigate the charge-carrier mobility and crystal energy of chiral [6]helicene in the paper. The purpose of this work was to investigate the effects of molecular packing on charge-carrier mobility, an important aspect of organic semiconductor performance.

Utilising sophisticated crystal structure prediction methods, the researchers examined the lattice-energy structure of [6]helicene. They explained why a racemate structure was not observed experimentally and successfully replicated the enantiopure crystal structure that was observed in the experiment. Through the analysis of the energy-structure-function landscape, they evaluated differences in electron and hole mobilities among various packing motifs. According to the study, the highest calculated electron mobility, which was found in a particular packing motif, was 2.9 cm² V⁻¹ s⁻¹, assuming a reorganisation energy of 0.46 eV. Furthermore, the largest estimated hole mobility, found in helicenes arranged in a herringbone pattern, was 2.0 cm² V⁻¹ s⁻¹.

Our results show that the packing motifs with high charge-carrier mobility and energetic favorability are not readily apparent, underscoring the significance of computational methods in forecasting the solid-state configurations and characteristics of organic semiconductors. This paper offers a comprehensive framework for solid-state structure and property prediction of chiral organic semiconductors using computational simulations. It emphasises the value of energy landscape exploration and crystal structure prediction in creating novel molecules for organic electronics, which I will need to use to direct the first stages of my research.

“Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality”

This study investigates the effects of molecular chirality on the electronic characteristics of organic semiconductors, concentrating on molecules with helicoidal chirality such as 1-aza[6]helicene. The work demonstrates the important impact of chirality on charge mobility by showing that, depending only on the ratio of enantiomers constituting the molecular crystal structure, organic field-effect transistors (OFETs) composed of helically chiral molecules can display hole mobility differences of up to 80 times. This significant difference highlights the significant impact of molecular chirality on the characteristics of charge transport.

When the researchers compared enantiopure (single handedness) and racemic (1:1 mixture of left- and right-handed) films, they noticed significant differences in thin-film morphology and photophysical characteristics. Higher mobility and improved charge transport were demonstrated by enantiopure films. The study explains how the chiral nature of the molecules affects the packing structure, electronic coupling, and reorganisation energy—all important factors in determining charge mobility—by combining computational modelling with experimental data.

According to the research, taking advantage of molecular chirality in organic semiconductors may help create organic electronic devices like light-emitting diodes, solar cells, and transistors that are more efficient. This study offers important insights on optimising charge mobility when studying helicene derivatives and is crucial to comprehending the potential application of chirality-induced spin selectivity (CISS) in the design of highly efficient organic electronic devices.

### Summaries of Recent Papers on Helicene Radicals:

“Illuminating the Property Space in Crystal Structure Prediction Using Quality-Diversity Algorithms”

A new method for investigating the crystal structure prediction using Quality-Diversity (QD) algorithms is presented by Wolinska et al. (2024). In contrast to conventional optimisation techniques, which only look for the best answers, QD algorithms look for a variety of excellent answers. This thorough investigation offers a clearer picture of the property space by pointing out several viable options in addition to the best ones. Using QD algorithms can greatly improve my research on helicene radicals by allowing me to investigate more possible structures. An extremely exciting development is that this approach might be very helpful in guaranteeing a comprehensive exploration of helicene derivatives and identifying multiple candidates with desirable electronic and spintronic properties, which might have been missed using traditional methods.

“Insights into the Magnetism and Phase Transitions of Organic Radical-Based Materials”

Important information about the magnetism and phase transitions of materials based on organic radicals is given by Deumal et al. (2021). In order to gain a better understanding of the mechanisms underlying these processes, this research uses both experimental data and computational models to investigate the magnetic properties and phase transitions of these materials. This paper provides detailed insights that can guide strategies to improve stability and control over the magnetic behaviour of helicene radicals, making them more useful as functional advanced electronic devices. It will also provide food for thought when suggesting candidates for synthesis.

“Long Spin Diffusion Lengths in Doped Conjugated Polymers Due to Enhanced Exchange Coupling”

The enhanced spin diffusion lengths in doped conjugated polymers are reported by Wang et al. (2019). In order to clarify the mechanisms underlying the observed properties, the study combines theoretical and experimental methods and attributes this improvement to enhanced exchange coupling. These results are very pertinent to my research on helicene radicals; similar doping approaches may improve the transport and spin coherence of helicene radicals, increasing their usefulness for spintronic devices. This paper will be important to consult when trying to maximise spin diffusion for possible suggested molecules.

“Design and Applications of Single-Component Radical Conductors”

Yuan et al. (2021) cover a wide range of design concepts and uses for standard single-component radical conductors in their thorough review. This paper focuses on different approaches to improve these materials' stability and electrical conductivity. This work is crucial because it provides guidelines for the initial design and modelling of molecules for simulations. The strategies discussed can be directly applied to helicene radicals to enhance their charge transport properties.

A summary of relevant papers in machine learning/neural networks:

Genetic Algorithms and Neural Networks in Molecular Design:

Using genetic algorithms (GA) in conjunction with neural networks (NN) offers a potent way to optimise molecular designs. This method effectively navigates the large molecular space by utilising the predictive strength of NNs and the exploratory capabilities of GAs. Neural networks forecast the characteristics of these candidates, such as charge carrier mobility and spin filtering capabilities, while genetic algorithms produce a variety of molecular candidates (Elton et al., 2019). This combination makes it possible to explore chemical space more specifically, which is advantageous for the development of derivatives of helicene. The effectiveness of finding promising helicene candidates with desired electronic properties can be greatly increased by using such a method.

JANUS: Efficient Genetic Algorithm for Molecular Discovery:

A genetic algorithm that prioritises sample efficiency, known as JANUS, makes it easier to find the best solutions with fewer evaluations. Through the use of JANUS in the computational search for helicene radicals, scientists can find molecules with ideal electronic properties more quickly. Because of its efficiency, the algorithm can expedite the discovery phase of molecular design projects by saving time and money on computation (Gallarati et al., 2023).

STONED-SELFIES: Novel Molecule Generation:

To create new molecules, STONED-SELFIES combines molecular representation methods known as SELFIES (Self-Referencing Embedded Strings) with genetic algorithms (Greenstein et al., 2023). Exploring the chemical space of helicene radicals requires generating molecular candidates with greater diversity, which is what this method does. STONED-SELFIES offers a strong framework for finding promising helicene radicals with distinctive properties by forecasting the electronic and spintronic characteristics of these candidates. This method is especially helpful in producing a broad variety of molecular structures, which raises the possibility of finding high-performance materials.

Deep Learning and Optimization Techniques in Molecular Design:

Elton et al.'s (2019) review emphasises how deep learning methods are used in molecular design. The transformative potential of deep learning in the field of property prediction and molecule generation is highlighted in this extensive review, which covers multiple architectures and methods. The prediction accuracy of the electronic properties of helicene radicals can be greatly improved by incorporating deep learning models into the research. Through the use of sophisticated computational models and large datasets, this integration makes it easier to identify high-performance candidates by revealing patterns and insights that conventional methods might miss.

### Quantum-Inspired Cluster Expansion:

### A quantum-inspired cluster expansion method was presented by Choubisa et al. (2023) to expedite the search for ideal materials. This technique efficiently explores the chemical space to find candidates with superior spin filtering and conductivity properties, using quantum-inspired algorithms. Through the application of these algorithms, scientists can further optimise the exploration of helicene derivatives and may find materials with remarkable spintronic and electronic characteristics.

### Genetic Algorithms for Homogeneous Catalysts:

### In Gallarati et al.'s (2023) paper, the efficiency and efficacy of using genetic algorithms to find homogeneous catalysts are discussed. The techniques discussed in this paper can be modified to maximise helicene radical design and guarantee the identification of molecules possessing the required electronic characteristics. Researchers can systematically explore the parameter space and find the best molecular structures that satisfy particular performance requirements by using genetic algorithms.

### Best Practices for Genetic Algorithms:

### Guidelines for the efficient application of genetic algorithms in molecular discovery are presented by Greenstein et al. (2023). In order to maximise the effectiveness and precision of genetic algorithms, the paper highlights the significance of parameter tuning and evaluation techniques. The genetic algorithms for the study of helicene radicals will be optimised for finding high-performance molecules if these best practices are put into practice. This strategy will improve the molecular discovery process's robustness and dependability.

### Data-Driven Models and Bayesian Optimization:

### Data-driven models were presented by Greenstein and Hutchison (2022) to forecast the efficiency of organic solar cells with non-fullerene acceptors. The efficiency of helicene-based organic semiconductors can be predicted using these models, which can help identify good candidates for additional research. Researchers can obtain insights into the factors influencing the performance of helicene materials by utilising data-driven approaches.

### Constrained Bayesian Optimization:

### In 2020, Griffiths and Hernández-Lobato investigated automatic chemical design using Bayesian optimisation techniques. By concentrating on improving molecular characteristics, this strategy provides a potent instrument for adjusting helicene radical characteristics. Helicene-based materials perform better overall when molecules with the best charge transport and spin coherence are identified through constrained Bayesian optimisation.

### Genetic Algorithms for Molecule Generation:

### Tripp and Hernández-Lobato (2023) talk about how good genetic algorithms are as starting points for creating molecules. A comprehensive exploration of the chemical space is ensured by the robust method of generating and optimising helicene derivatives offered by genetic algorithms. These algorithms can find candidates with desired electronic properties by systematically varying molecular structures.

### Quality-Diversity Algorithms:

The application of quality-diversity algorithms to enlighten the property space in crystal structure prediction is highlighted by Wolinska et al. (2024). By using these algorithms on helicene derivatives, it is possible to find a variety of excellent structures and raise the likelihood of finding compounds with remarkable electronic characteristics. The utilisation of quality-diversity algorithms in the exploration process results in a more thorough comprehension of the possible performance of various helicene configurations.

Considering these various methods, I will be able to optimise a strong and effective computational technique for simulating and modelling radical Helicenes by incorporating some of these cutting-edge computational techniques into my research. In order to identify possible uses for all these innovative techniques, I will need to keep a careful watch on them all while conducting my research. It will be helpful to have a working knowledge of them all in my toolbox, even though it is unlikely that I will need or utilise them all.

### Research Proposal: A computational investigation of novel radical Helicenes, optimising Spin Filtering and Coherence to identify promising synthetic targets

Advanced organic semiconductors with improved charge mobility and spin filtering capabilities can be developed via the integration of stable neutral radicals and helical chirality in helicenes. My research proposal therefore describes a computational method to study new chiral helicenes with the goal of finding good candidates for synthesis that have better semiconductor properties, especially in terms of spin coherence and charge carrier and hole mobility.

This work aims to develop and characterise novel chiral helicenes by combining the properties of stable neutral radicals with those of helicene. The purpose of these helicenes is to improve spin filtering and charge carrier mobility. I will forecast the crystal structures and carrier mobilities of known and new helicene derivatives by developing and verifying computational models. In addition, I will look into these helicenes' spin coherence and spin-selective transport characteristics. In the end, I want to build a computational pipeline that will automate the simulation and analysis of helicene properties.

Electronic structure calculations and crystal structure predictions will be the first step in my research, using computational software packages like Gaussian, VASP, and CRYSTAL. These instruments will precisely simulate the electronic characteristics and forecast the ideal crystal configurations for helicene radicals. The techniques taken from Rice et al. (2018) will be crucial, with an emphasis on lattice-energy landscape prediction to identify stable crystal structures of helicenes and model potential energy surfaces. I will apply these approaches to new helicene-radical derivatives, starting with well-studied molecules such as [6]helicene, to guarantee thorough investigation of the chemical space.

I will use Density Functional Theory (DFT) and Marcus theory to assess charge carrier mobility. By calculating electronic coupling constants and reorganisation energies, electron and hole mobilities will be determined. The helicenes' electronic structures and reorganisation energies will be thoroughly explained by DFT calculations. I will model the electronic characteristics and charge transport processes in various crystal packing configurations using VASP (Elton et al., 2019). To simulate the properties of charge transport, charge hopping models, like Kinetic Monte Carlo simulations, will be used, taking into account the impact of various molecular packing motifs on mobility.

In terms of spin filtering and coherence, I will use computational techniques to simulate spin-dependent electronic transport, with particular attention to the effect of molecular chirality on spin coherence. The CISS effect will be modelled with techniques from Gaussian and VASP, which is important to comprehend the spin filtering properties of the helicene radicals. The spin polarisation of electrons travelling through the helicenes will be predicted and spin transport properties will be analysed using spin-polarized density functional theory (SP-DFT).

All computational tools and techniques will be integrated through the creation of an automated Python-based workflow, allowing for smooth simulation and analysis. To guarantee a streamlined and effective procedure, scripts for data analysis, simulation execution, and input generation will be put into place. The workflow parameters will be optimised using machine learning algorithms, increasing the simulations' precision and effectiveness (Greenstein et al., 2023).

A screenshot of a computer

Description automatically generatedTo guarantee accuracy and dependability, my computational models will be validated using experimental data from the literature. To improve the models' predictive power, computational parameters will be optimised using Bayesian optimisation techniques and data-driven models (Griffiths & Hernández-Lobato, 2020). The automated workflow will be used for high-throughput screening to create a library of helicene derivatives and predict their electronic and spintronic properties. To find candidate molecules with the desired properties, the predicted properties will be compared with experimental readings and other simulated molecules. Given the known conductivity of the Blatter-type and bisdithiazolyl radical groups presented on the right (Brandt, unpublished), I will first look into the variations displayed of these, which should be a good starting point to gather initial data.

A screenshot of a computer

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Once I have assessed how the project is transpiring and having established a workflow, I will additionally investigate molecules based on the boron spiro-biphenalenyl structure (see left), which has been reported to be conductive and predicted to have increased conductivity were the pi delocalisation in the molecule to be increased.

This research aims to systematically explore and optimise the chemical space of helicene radicals by integrating these computational methods and approaches. This will allow efficient prediction of electronic and spintronic properties, which will ultimately guide the synthesis of high-performance helicene-based organic semiconductors.

The creation and validation of precise computational models for forecasting the characteristics of helicene radicals, the prediction and characterization of novel helicene molecules with improved charge carrier mobility and spin filtering properties, and the implementation of an automated computational pipeline for high-throughput screening of helicene derivatives are among the anticipated results of this research. Furthermore, this work will shed light on the mechanisms underlying coherence and spin-selective transport in chiral helicenes.

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