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Research Article

DFT-Based Molecular Analysis of Imidazole Derivatives as Additives to Enhance Ionic Conductivity in Polymer Electrolyte Membranes

Analisis Molekuler Berbasis DFT terhadap Turunan Imidazol sebagai Aditif untuk Meningkatkan Konduktivitas Ionik dalam Membran Polimer Elektrolit

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Abstract

The demand for efficient and stable lithium-ion batteries has driven research on advanced polymer electrolyte membranes (PEM) with improved ionic conductivity. This study investigated imidazole and its derivatives as additives in PEM to enhance battery performance. Using Density Functional Theory (DFT) with the def2-TZVP basis set, key quantum parameters such as HOMO-LUMO energies, energy gap (ΔEgap), electronegativity (χ), softness (σ), electron transfer fraction (ΔN), and net electrophilicity (Δω) were analyzed. Results showed that imidazole derivatives with electron-withdrawing groups, like acrylate and tosyl, had lower E_{LUMO} and smaller ΔE_{gap}, improving lithium ion (Li^+) interactions and mobility within the polymer matrix. Additionally, compounds with high χ and σ, such as BTIM and BZIM, enhanced ion stabilization and transport, leading to better electrolyte performance. Thus, modifying imidazole structures through specific substitutions is a promising approach to optimize PEM, supporting the development of more efficient and stable lithium-ion batteries.

Keywords: DFT; imidazole; ionic conductivity; lithium-ion battery; PEM

Abstrak

Permintaan akan baterai ion litium yang efisien dan stabil telah mendorong penelitian mengenai membran elektrolit polimer (PEM) yang memiliki konduktivitas ionik lebih tinggi. Studi ini menyelidiki imidazol dan turunannya sebagai aditif dalam PEM untuk meningkatkan kinerja baterai. Dengan menggunakan Teori Densitas Fungsional (DFT) dan basis set def2-TZVP, berbagai parameter kuantum, seperti energi orbital HOMO-LUMO, celah energi (ΔEgap), keelektronegatifan (χ), kelembutan (σ), fraksi transfer elektron (ΔN), dan elektrofilisitas bersih (Δω), dianalisis. Hasil menunjukkan bahwa turunan imidazol dengan gugus penarik elektron, seperti akrilat dan tosyl, memiliki E_{LUMO} *yang lebih rendah serta* ΔEgap *yang lebih kecil, sehingga meningkatkan interaksi dan mobilitas ion litium (*Li^+*) dalam matriks polimer. Selain itu, senyawa dengan nilai χ dan σ yang tinggi, seperti BTIM dan BZIM, meningkatkan stabilisasi dan transportasi ion, sehingga memperbaiki kinerja elektrolit. Oleh karena itu, modifikasi struktur imidazol melalui substituen tertentu menjadi strategi yang menjanjikan untuk mengoptimalkan PEM, mendukung pengembangan baterai ion litium yang lebih efisien dan stabil.*

Kata kunci: *Imidazol, PEM, Konduktivitas ionik, DFT, Baterai ion litium*

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1. Introduction

In recent decades, polymer electrolyte materials (PEM) development has become a central focus in the lithium-ion battery industry. Concerning the matter, conductive and stable polymer electrolytes are crucial in enhancing battery efficiency and durability. Following this, one promising approach can be modifying electrolyte membranes with additives that can improve mechanical properties and ionic conductivity [1]. Heterocyclic aromatic organic compounds such as imidazole and its derivatives hold significant potential in this application. This is particularly due to their ability to act as plasticizers and proton donors, which can accelerate ion transport within the polymer matrix [2]. Therefore, further exploration of the activity and mechanisms of these compounds in improving polymer electrolyte performance is essential.

Imidazole is a heterocyclic compound containing two nitrogen atoms in its aromatic ring structure. These atoms impart unique properties, such as moderate acidity and interaction ability with lithium ions and other anions [3]. In electrolyte systems, imidazole can function as a proton-conducting agent. This agent enhances hydrogen ion mobility, improving charge transfer efficiency within the polymer membrane. Furthermore, imidazole derivatives with various substituents can be utilized to control the physical and chemical properties of the compound, such as solubility, thermal stability, and interaction with the polymer matrix [4]. Thus, a critical aspect of this research is a deeper understanding of the relationship between molecular structure and the effectiveness of imidazole-based additives in enhancing ionic conductivity.

Previous studies have shown that the use of imidazole compounds as additives in polymer electrolyte membranes could significantly improve proton conductivity. For instance, Mu et al. [5] found that incorporating 4-(1H-imidazol-1-yl) benzaldehyde as a monomer in polymer synthesis increased proton conductivity to 50.2×10^{-3} S/cm. This modification also resulted in stable cycle performance for 173 hours, demonstrating its potential as an electrolyte membrane. Additionally, Liu et al. [6] developed a novel double-network hydrogel-polymer electrolyte (DNHPE) based on polyvinyl alcohol (PVA), polyacrylamide (PAM), and 1-ethyl-3-methylimidazolium tetrafluoroborate ([EMIM][BF_4]). The electrolyte exhibited ionic conductivity up to 9.34 S/m, stretchability (650%), and thermal stability, making it suitable for lithium-ion battery and supercapacitor technologies.

This study addressed a critical gap by investigating the influence of specific electron-withdrawing substituents (acrylate and tosyl) on the electronic structure and lithium ion coordination in imidazole derivatives. Unlike prior works that focused on general reactivity or proton transport [5, 6], our approach systematically investigated DFT-based quantum descriptors (E_{LUMO}, ΔE_{gap}, softness, and electrophilicity) to inform the rational design of PEM additives.

Quantum computational methods, particularly Density Functional Theory (DFT), have become invaluable tools for exploring the electronic properties and molecular structures of chemical compounds [7]. DFT enables a detailed analysis of how the molecular structure of imidazole and its derivatives influence proton conductivity and other ionic properties. By understanding the

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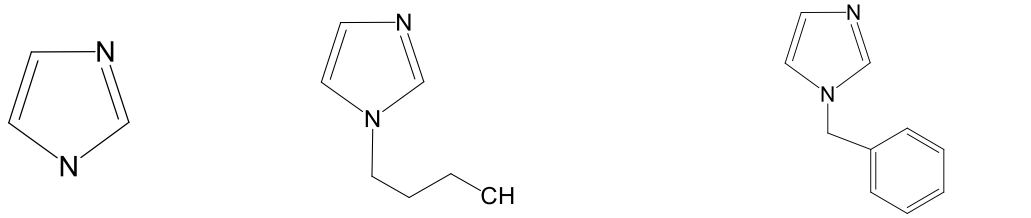
relationship between molecular structure and ionic activity, more efficient additive compounds can be designed for lithium-ion battery applications. Kumar & Venkatnathan [8] used DFT to demonstrate that proton transport requires overcoming energy barriers and that imidazole molecular rotation plays a more significant role in determining the rate of proton conduction than the proton hopping mechanism itself.

This study employed a DFT-based approach to explore the potential activity of imidazole and its derivatives as additives in PEM. The analysis focused on the relationship between molecular structure and electronic properties and their contribution to enhancing proton conductivity. One of the key parameters examined was softness (σ), which correlates with the compound's ability to support charge transport in electrolyte systems [9]. Through quantum mechanical modeling, this research aimed to provide a deeper understanding of the factors influencing the effectiveness of imidazole as an electrolyte additive. These findings offer new insights into the design of more efficient electrolyte materials. Furthermore, this work introduced a comparative analysis of DFT-derived parameters such as softness (σ), net electrophilicity (Δω), and electron transfer fraction (ΔN). These parameters have not previously been examined collectively in the context of imidazole-based PEM additives [1][5], thereby contributing a novel methodological approach.

2. Research Methods

2.1 Materials and Tools

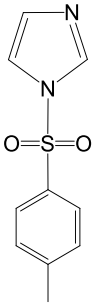
This research employed a computer equipped with an Intel i5-3317U processor, a CPU speed of 1.7 GHz, and 8 GB of RAM. Computational calculations were performed using the Orca software version 4.2.1, while the design of organic compound structures was visualized using Avogadro software. Analysis and interpretation of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) were conducted using IboView software.



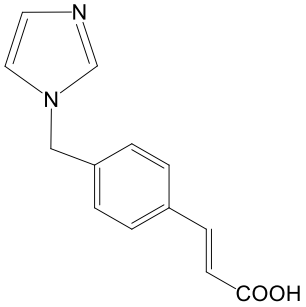
[A], imidazole **IM**

[B], 1-butyl-1H-imidazole **BTIM**

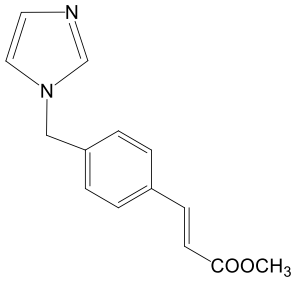
[C], 1-benzyl-1H-imidazole **BZIM**



[D], 1-tosyl-1H-imidazole **TSIM**



[E], (E)-3-(4-((1H-imidazole-1-yl)methyl)phenyl)acrylic acid **IMMP**



[F], (E)-methyl 3-(4-((1H-imidazole-1-yl)methyl)phenyl)acrylate **MIMMP**

Figure 1. Molecular structures of imidazole and its derivatives

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2.2 Experimental Procedures

In this study, quantum chemical calculations were performed using Orca version 4.2.1 as the primary analysis tool. Initial molecular geometries were obtained from PubChem database (https://pubchem.ncbi.nlm.nih.gov/), which provides comprehensive structural and molecular information. After obtaining the appropriate molecular structures, calculations were performed using the DFT with Becke's three-parameters Lee-Yang-Parr (B3LYP) method and the def2-TZVP basis set [10]. Visualizations of the molecular structures of imidazole and its derivatives are detailed in Figure 1.

The distributions of molecular orbitals, specifically the HOMO and LUMO, were analyzed to understand the electronic properties of imidazole and its derivatives [11]. Orbital visualizations were performed using IboView software to map electron distribution and identify regions potentially involved in ionic interactions. HOMO (E_{HOMO}) and LUMO (E_{LUMO}) energies were estimated to determine the energy gap (ΔE_{gap}), which correlates with the stability and reactivity of the compounds.

Several quantum parameters were examined to evaluate the potential of imidazole and its derivatives as additives in electrolyte membranes. These parameters included energy gap, electronegativity, hardness, softness, electron transfer fraction, and net electrophilicity.

The energy gap (ΔE_{gap}), which describes electronic stability and the tendency for charge transfer [12], was computed using equation 1. Electronegativity (χ), which represents a molecule's ability to attract electrons, was determined with equation 2 based on DFT. From equation 2, E is the electronic energy, N is the number of electrons in the system, and v(r) is the external potential from atomic nuclei. The electronegativity value can be further calculated using equation 3, which defines χ as the average of ionization energy (I) and electron affinity (A) [13]. The I value was attained from the HOMO energy ($I = -E_{HOMO}$), while the A value was obtained from the LUMO energy ($A = -E_{LUMO}$).

$$\Delta E_{gap} = E_{LUMO} - E_{HOMO} \quad \text{.....(1)}$$

$$\chi = \left(\frac{\partial E}{\partial N}\right)_{v(r)} \quad \text{.....(2)}$$

$$\chi = \frac{I+A}{2} \quad \text{.....(3)}$$

$$\eta = \frac{I-A}{2} \quad \text{.....(4)}$$

$$\sigma = \frac{I}{\eta} \quad \text{.....(5)}$$

$$\Delta N = \frac{(\chi_M - \chi_{mol})}{2\,(\eta_M - \eta_{mol})} \quad \text{.....(6)}$$

$$\Delta\omega = \omega^+ - \omega^- \quad \text{.....(7)}$$

Hardness (η), which designates a molecule's resistance to changes in electron distribution, was computed using equation 4. Softness (σ) is the inverse of hardness, indicating the ease with which a molecule can undergo polarization, estimated through equation 5 [14]. Electron transfer fraction (ΔN), which defines a compound's ability to transfer electrons to a metal or another system, was calculated using equation 6 [15]. χ_M dan η_M are the electronegativity and hardness of the metal (e.g., lithium), respectively, while χ_{mol} and η_{mol} are the electronegativity and hardness of the imidazole compound or its derivatives. In this study, the absolute electronegativity (χ) of lithium (Li) was determined to be 4.82

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eV, while the hardness (η) was 0 eV. Net electrophilicity (Δω) is the difference in electrophilicity index between donor and acceptor compounds in a system, determined through equation (7) [16]. Electron-accepting power (ω^+) was obtained from $\omega^+ = \frac{(I+3A)^2}{16(I-A)}$, while electron-donating power (ω^-) was attained from $\omega^- = \frac{(3I+A)^2}{16(I-A)}$.

3. Results and Discussion

This study employed DFT with the def2-TZVP basis set to analyze the electronic properties of imidazole and its derivatives. This basis set was chosen for its ability to accurately describe electron correlation and exchange effects, making it suitable for predicting the properties of complex molecules. This approach enables in-depth analyses of molecular structure, charge distribution, orbital energies, and interactions with lithium ions [8]. This method is also computationally efficient, enabling simulations of medium to large-sized molecules without sacrificing accuracy [17][18].

This study focused on internal substituent variation within the imidazole framework to ensure consistent comparison. Although other heterocycles like triazoles or pyridines were not analyzed in this study, the well-established proton-donating ability and electronic tunability of imidazole justify its selection [2][4]. Future work may include broader comparisons.

Figure 1 illustrates the molecular structures of selected imidazole derivatives, selected based on variations in substituent type and position. BTIM has an alkyl chain, while BZIM and TSIM contain aromatic rings promoting π-stacking, and IMMP and MIMMP carry acrylates that facilitate lithium ion binding via conjugated electron systems [19].

The Frontier Molecular Orbital (FMO) approach was employed to evaluate molecular reactivity and stability through calculations of the HOMO and LUMO energies. HOMO energy (E_{HOMO}) indicates a molecule's tendency to release electrons, while LUMO energy (E_{LUMO}) describes its ability to accept electrons [11]. Imidazolium cations, formed from imidazole compounds, have a delocalized positive charge on their ring. The energy gap (ΔE_{gap}) between HOMO and LUMO, calculated using the Fukui equation (equation 1), correlates with the ease of electron transfer and molecular stability [20]. The calculated E_{HOMO}, E_{LUMO}, and ΔE_{gap} values are presented in Table 1.

The lowest LUMO energy (E_{LUMO}) indicates a molecule's tendency to accept electrons from higher-energy species. Imidazolium cations with low E_{LUMO} exhibit strong electrophilic properties, facilitating interaction with lithium ions and distributing these ions within the polymer matrix [9]. Based on Table 1, the order of E_{LUMO} is Compounds **[E] < [F] < [D] < [C] < [B] < [A]**. Additionally, the smaller energy gap (ΔE_{gap}) values for derivatives **[E]** and **[F]** denote higher chemical reactivity. This is related to the molecular structure containing electron-withdrawing substituents, such as acrylate groups, which enhance electrophilic properties and interaction with lithium ions [21]. Consequently, these structural features promote improved charge accommodation and lower ion migration barriers across the PEM matrix.

The FMO (HOMO and LUMO) distributions of imidazole and its derivatives, depicted in Figure 2, demonstrate dominant p-orbital

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contributions. These electron-rich p-orbitals facilitate critical π-π interactions [12] and enhance coordination with lithium ions, directly impacting ionic conductivity within polymer electrolyte membranes.

Electron-withdrawing substituents, including acrylate and tosyl groups, substantially reduce LUMO energy levels, thereby improving electrophilicity and electron-accepting capacity. Such substituents also modify molecular geometry through conjugated π-systems or sulfonyl moieties, which promote greater orbital overlap and strengthen lithium ion coordination. These effects correlate with enhanced π–π stacking interactions and shorter coordination distances, contributing to higher ionic mobility [11][22].

Beyond electronic effects, substituents such as benzyl, tosyl, and acrylate introduce structural distortions in the imidazole ring, increasing non-planarity and extending conjugation. These conformational changes improve lithium ion coordination by expanding the accessible surface area while minimizing steric hindrance, contributing to more effective ion stabilization and transport [12][23]. Analysis of other quantum parameters, such as electronegativity (χ), hardness (η), softness (σ), electron transfer fraction (ΔN), and net electrophilicity (Δω), provides a deeper understanding of the additive properties of imidazole and its derivatives. These results are presented in Table 2.

Table 1. Quantum parameters of imidazole and its derivatives using the DFT with the B3LYP method and the def2-TZVP basis set

Parameters	Compounds					
	[A]	[B]	[C]	[D]	[E]	[F]
E_{HOMO} (eV)	-6.359	-6.155	-6.185	-6.656	-6.307	-6.283
E_{LUMO} (eV)	0.452	0.397	-0.803	-1.905	-2.218	-2.182
ΔE_{gap} (eV)	6.811	6.552	5.382	4.751	4.090	4.101

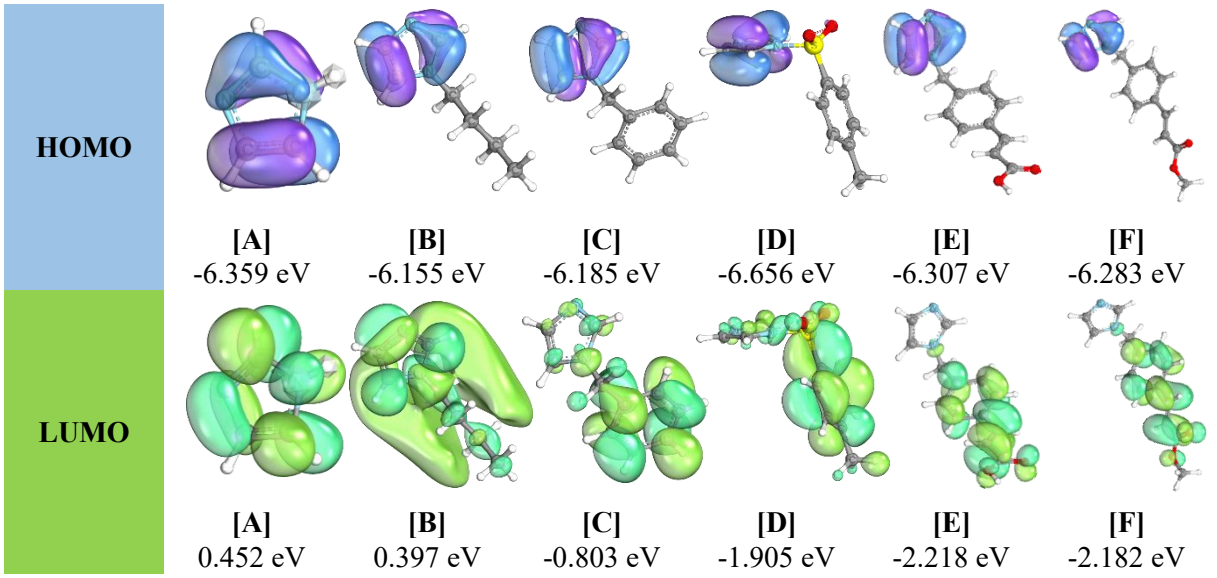

Figure 2. FMO diagrams of imidazole and its derivatives

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Table 2. Quantum parameter calculations of imidazole and its derivatives

Parameters	Compounds					
	[A]	[B]	[C]	[D]	[E]	[F]
I (eV)	6.359	6.155	6.185	6.656	6.307	6.283
A (eV)	-0.452	-0.397	0.803	1.905	2.218	2.182
χ (eV)	2.954	2.879	3.494	4.280	4.262	4.233
σ (eV)	0.294	0.305	0.372	0.421	0.489	0.488
ΔN (eV)	0.274	0.296	0.246	0.114	0.136	0.143
Δω (eV)	-0.026	2.855	3.523	3.888	2.977	3.048

According to Koopmans' theory, the ionization energy (I) of a molecule can be approximated as the negative of E_{HOMO}, while the electron affinity (A) is the negative of E_{LUMO}. These parameters were computed through equations (3) and (4). This theory assumes that the molecular orbital structure does not change when electrons are removed or added [20]. Electronegativity (χ) reflects the ability of an atom or compound to attract electrons. In polymer electrolyte additives, compounds with appropriate electronegativity can enhance the interaction of lithium ions with functional groups on the additive, thereby improving stability and ionic conductivity [24]. Based on Table 2, the order of electronegativity is Compounds **[D] > [E] > [F] > [C] > [A] > [B].** Compounds **[D], [E],** and **[F]** had higher electronegativity values considered due to the presence of electron-withdrawing substituents such as tosyl and acrylate groups. These substituents enhance electron-attracting ability and interaction with lithium ion [22]. In contrast, compounds **[A]** and **[B]** had lower electronegativity values due to their simple molecular structures and lack of electron-withdrawing substituents.

Softness (σ), the inverse of hardness (η), describes a molecule's ability to undergo polarization, which is essential for interactions with lithium ion in PEM. According to Hard-Soft Acid-Base (HSAB) theory, lithium ions are hard acids, so their interaction with imidazole-based additives is influenced by molecular softness [14]. Molecules with high softness are more flexible in adjusting electron distribution, enhancing lithium ion mobility and ionic conductivity in PEM. Based on Table 2, the order of softness is **[A] < [B] < [C] < [D] < [F] < [E]**. It reveals that Compounds **[F]** and **[E]** exhibited superior softness values, enhancing polarization under an electric field and improving lithium ion mobility [23]. These electronic trends confirm the strategic importance of substituent selection for PEM design.

In lithium-ion battery systems, PEM serves as the medium for lithium ion transport between the cathode and anode. The mechanism of lithium ion conduction in PEM involves two main processes. The first is ion transfer through the polymer matrix, and the second is electron transfer through interactions with additive molecules incorporated into the membrane [25]. The Electron transfer fraction (ΔN) represents the additive's ability to transfer electrons to lithium ion. A positive ΔN value denotes a molecule's tendency to act as an electron donor. According to Charge Transfer Theory, this interaction can enhance lithium ion mobility and proton conductivity in PEM [5]. Based on Table 2, the order of ΔN is Compounds **[B] > [A] > [C] > [F] > [E] > [D]**. Compounds with

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high ΔN, such as **[B]** and **[A]**, can be attributed to the uniform electron distribution in the simple aromatic ring of imidazole **[A]** and the presence of electron-donating butyl substituents in **[B]**, which increase its overall electron density. This makes them more effective in donating electrons to lithium ions, facilitating interaction and ion transport [18][26].

Net electrophilicity (Δω) defines a compound's strength as an electrophile [16], essential for understanding interactions with lithium ions in polymer electrolytes. Compounds with appropriate electrophilicity can regulate ion interactions and enhance the stability of polymer electrolyte membranes [27][28]. Based on Table 2, the order of Δω is Compounds **[E] > [F] > [D] > [C] > [A] > [B]**. High Δω values (above 1.5 eV) support the potential of imidazole and its derivatives as additives in PEM [29].

Although this study is theoretical, the findings align with experimental data from imidazole-based systems [5]. For instance, Liu et al. [6] demonstrated that acrylate-functionalized imidazole derivatives achieved high ionic conductivities (up to 9.34 S/m), supporting our predictions based on high softness and favorable ΔN values. This correlation underscores the practical relevance of the computed quantum descriptors.

The theoretical trends further align with established experimental results, including the observation by Zhang et al. [19] of improved protective properties and enhanced ion interactions in TSIM and MIMMP derivatives. These consistencies emphasize the critical influence of substituent architecture on functional performance despite the current lack of direct experimental validation in our work.

While the def2-TZVP basis set provides reliable electronic structure modeling, we acknowledge that incorporating explicit solvent effects and molecular dynamics would offer more comprehensive insights. Nevertheless, the strong agreement with empirical data supports the robustness of our findings [5][19], warranting future investigations combining Density Functional Theory – Molecular Dynamics (DFT-MD) approaches with experimental characterization.

This study establishes a fundamental understanding of the relationship between the molecular structure and ionic conductivity performance of imidazole-based PEM additives through systematic DFT analysis. The demonstrated correlation between molecular architecture and conduction enhancement offers a strategic framework for designing next-generation electrolyte materials, suggesting promising directions for future theoretical and experimental studies.

4. Conclusion

The DFT-based investigation revealed that imidazole derivatives bearing electron-withdrawing substituents—especially acrylate and tosyl groups—exhibited enhanced electronic characteristics favorable for lithium ion coordination and transport within PEM. The low LUMO energies, narrow energy gaps, and elevated softness values observed in compounds such as MIMMP and IMMP reflect high electrophilicity and polarizability, which are critical for efficient lithium ions migration across the polymer matrix. These molecular traits are strongly associated with improved ionic conductivity, as demonstrated by quantum descriptors including ΔE, σ, ΔN, and Δω.

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Furthermore, the ease of synthesis via well-established acrylation and tosylation methods supports the practical implementation of these derivatives in experimental PEM systems. These results demonstrate a predictive strategy for optimizing additives, thereby facilitating the development of high-performance PEM materials for next-generation applications.

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