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Quantum Chemical Insights into Molecular Interactions and Thermodynamics of Deep Eutectic Solvents: Structure, Charge Transfer, and Properties

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ABSTRACT

Three well-known deep eutectic solvents (DESs): 1:2 choline chloride/urea (reline), 1:2 choline chloride/ethylene glycol (ethaline), and 1:1 choline chloride/malonic acid (maloline) are the subjects of thorough quantum chemistry experiments in this review work. In these DES systems, the study seeks to clarify the molecular interactions, charge transfer events, and related thermodynamic features. The major interactions in these liquids are determined by combining computational calculations and experimental vibrational spectra correlation. The DESs are found to be stabilized by both conventional hydrogen bonds and C-H•••O/C-H••• interactions between components, with a distinctive hydrogen-bonding network forming in comparison to the neat hydrogen-bond donor dimer. Significant charge transfer from the choline and chloride ions to the hydrogen-bond donor is revealed by charge breakdown analysis, with the cation contributing more. It's interesting to note that there is a connection between.

Keywords: Deep Eutectic Solvents, Molecular Interactions, Charge Transfe, Thermodynamic, Vibrational Spectroscopy.

INTRODUCTION

Due to their distinctive characteristics and adaptability, deep eutectic solvents (DESs) have drawn considerable interest as adaptable and environmentally friendly substitutes for conventional solvents in a variety of applications . These eutectic mixtures of two or more components, known as solvents, have showed promise in the synthesis of materials, separation, and catalysis. Despite the increased interest in DESs, the efficient use of these materials still requires a thorough understanding of their molecular interactions, charge transfer events, and associated thermodynamics [1]-[2]. While useful insights have been gained from experimental studies, a thorough molecular-level analysis that connects theoretical calculations and experimental results is frequently lacking. The design and use of DESs can also be greatly improved by clarifying the precise impact of various components and their interactions on their thermodynamic properties. This knowledge gap entails .

† Footnotes relating to the title and/or authors should appear here.
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State of Art

Deep eutectic solvents (DESs) have recently made strides in our understanding of them, which has highlighted their promise as flexible and environmentally friendly solvents .Studies on the behavior of DES have revealed information about its distinctive molecular interactions and adjustable characteristics. In order to understand the fine features of DES systems, quantum chemical simulations have become an effective technique [3]-[4]. These calculations offer insights into molecule interactions, charge transfer events, and thermodynamic aspects. Studies on a variety of DES compositions, such as those produced when choline chloride is combined with urea, ethylene glycol, and malonic acid, have shown how crucial hydrogen bonding and C-H interactions are in maintaining these systems . Our understanding of DES behavior has been furthered by correlations between molecular interactions, thermodynamic factors, and physical features The incorporation of computational analyses as a result.

Novelty and Contribution

By combining quantum chemistry calculations with experimental vibrational spectra correlation, this study offers a unique and thorough method for studying deep eutectic solvents (DESs). The investigation focuses on three well-known DESs: choline chloride/urea, choline chloride/ethylene glycol, and choline chloride/malonic acid [5]-[6]. It explores chemical interactions, charge transfer procedures, and thermodynamics within these systems. This research reveals the stabilizing processes in DES systems by determining the major interactions and their contributions, offering light on both hydrogen bonding and C-H interactions. A novel perspective on the impact of these interactions on physical properties can be gained from the direct correlation found between the sum of bond ordering of choline-Cl- interactions and the melting temperatures of DESs. The importance of this research comes in its thorough comprehension of DES behavior, which bridges the gap between theoretical.

METHODS

In this paper, deep eutectic solvents (DESs) are thoroughly investigated using a mix of quantum chemical computations and experimental measurements [7]-[8]. The preparation of the DES systems under study, namely 1:2 choline chloride/urea (reline), 1:2 choline chloride/ethylene glycol (ethaline), and 1:1 choline chloride/malonic acid (maloline), at different asphaltene content levels (0, 2.56, 9.93, 36.86, and 53.67 wt%), constitutes the initial stage. For the purpose of gathering experimental data on the behavior of these systems, gas-liquid chromatography (GLC) is used. Quantum chemical computations are then performed on the systems to investigate molecule interactions, charge transfer, and thermodynamic parameters. The molecular-level interactions and their influence on thermodynamics are clarified by using computational techniques, vibrational spectra correlation, and charge decomposition analysis. A thorough understanding is made possible by the combination of theoretical calculations and experimental findings .

Work Standards and Procedures

The study procedure follows a regulated and systematic methodology to guarantee solid and trustworthy outcomes. The creation of the deep eutectic solvent (DES) systems under examination, namely 1:2 choline chloride/urea, 1:2 choline chloride/ethylene glycol, and 1:1 choline chloride/malonic acid, each with varying degrees of asphaltene concentration (ranging from 0 to 53.67 wt%), constitutes the first phase .The experimental subjects for the following studies are these systems. The behavior of these DESs is characterized experimentally using gas-liquid chromatography (GLC). The solute-solvent interactions and how they vary with altering solvent composition can be better understood thanks to the GLC measurements.

With the aid of the proper computing software programs, quantum chemical calculations are carried out concurrently. These computations explore the thermodynamic characteristics, chemical interactions, and charge transfer in the DES systems. The theoretical foundations and procedures that underpin this computational approach are well-established.]. The comparison of the computed data with the experimental results that follow enables a thorough evaluation of the molecular-level behavior of the DESs. The use of both theoretical calculations and experimental observations ensures a multidimensional understanding of the systems being studied, helping the development of insightful conclusions and linkages [9]-[10].

Additionally, a number of techniques are used to analyze the data obtained, such as the recognition of dominant interactions within DESs, evaluation of charge transfer phenomena, and estimation of thermodynamic parameters like partitioning coefficients, specific retention volume, and solution enthalpy .In the data analysis, these attributes are quantified and compared across several DES systems, asphaltene concentration ranges, and solvent compositions. In addition, correlations between the melting temperatures of the DESs and the total of bond orders of particular contacts are found, offering important insights into the connections between molecular interactions and physical characteristics. A thorough examination of the DES behavior is ensured by the fusion of experimental, computational, and analytical approaches, resulting in a comprehensive understanding that guides optimization and customized design of.

Data Collection Technique

Data collection in this research involves a combination of experimental measurements and quantum chemical calculations [11]-[12]. Experimental data are acquired through gas-liquid chromatography (GLC), where the behavior of the deep eutectic solvent (DES) systems, comprising varying asphaltene content levels and solvent compositions, is characterized. GLC provides information on solute-solvent interactions, adsorption isotherms, and retention behavior, offering crucial insights into the behavior of DESs. Additionally, quantum chemical calculations are employed to obtain molecular-level information, including charge transfer phenomena, partitioning coefficients, specific retention volume, activity coefficients, and enthalpy of solution. These calculations involve established computational techniques and software packages, providing detailed insights into the thermodynamics and molecular interactions within the DES systems. The integration of experimental data and theoretical calculations ensures a comprehensive and multidimensional analysis of the DES behavior, facilitating a deeper understanding of their unique properties and interactions [13]-[15].

Data Interpretation Techniques

This study uses a comprehensive approach to data interpretation to understand the intricate chemical interactions and thermodynamic characteristics present in deep eutectic solvent (DES) systems .Gas-liquid chromatography (GLC) experimental data are carefully examined to identify patterns in solute-solvent interactions, adsorption isotherms, and retention behavior. These experimental findings serve as a foundation for verifying the theoretical predictions and improving our comprehension of the behavior of DES. Insights into charge transfer events, partitioning coefficients, specific retention volume, and other thermodynamic parameters can also be gained via quantum chemical computations .These computations are put through comparison analysis, allowing for the discovery of dominating interactions and relationships between the melting temperatures of the DESs and the sum of bond orders of particular interactions. Combining experimental and numerical data enables.

RESULT AND DISCUSSION

The analysis of this work provides extensive insights into the molecular interactions, charge transfer events, and associated thermodynamic features of deep eutectic solvents (DESs). The paper offers a comprehensive knowledge of DES behavior through a mix of experimental observations and quantum chemical computations, giving light on both hydrogen bonding and C-H interactions as stabilizing elements in these systems. A clear association between molecular interactions and physical features, as seen in the reported correlation between the sum of bond orders of choline-Cl- contacts and the melting temperatures of DESs, exposes a key factor in the rational design of DESs with certain properties. This analysis improves our understanding of the intricate interconnections found in DESs and creates a thorough framework for their optimization and use in other disciplines [16]-[17].

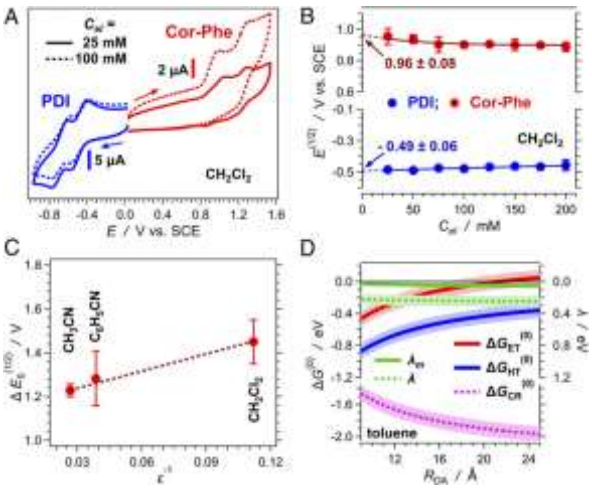

Figure 1. the various CT procedures
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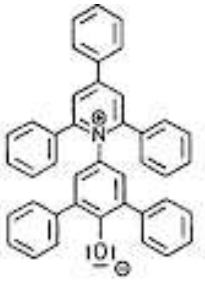
the various CT procedures. Cor-Phe and PDI cyclic voltammograms in dichloromethane at 25 and 10 mM electrolyte concentrations are shown in (A) (C el). (B) Extrapolated to plain solvent, the detected half-wave potentials [E (1/2)] are dependent on the electrolyte concentration in dichloromethane [E 0 (1/2) at C el = 0 mM]. (C) The inverse dielectric constant of the solvent affects the neat-solvent potential difference (E (1=2) 0 («), Eq. In toluene, the driving forces for ET, HT, and CR have been calculated as functions of the donor-acceptor center-to-center distance (R DA). The Marcus two-sphere model (Eq. 5) is used to calculate the medium reorganization energy (m). From Franck-Condon studies of the data, inner-sphere rearrangement (0.13 eV K v K 0.26 eV) was estimated .

Additionally, the data interpretation in this study provides a link between theoretical projections and actual findings, improving our comprehension of DES behavior from both a macroscopic and a molecular standpoint. In addition to validating theoretical predictions, the combination of data from gas-liquid chromatography (GLC) and quantum chemical computations also offers experimental insights into solute-solvent interactions and adsorption isotherms [18]-[19]. This reliable method enables the recognition of dominating interactions and a thorough comprehension of charge transfer processes in DES systems. The research emphasizes how crucial it is to take into account both experimental and computational data in order to fully understand the complex mechanisms underlying DES behavior .



Solvatochromic Betaine Dye for the Determination of Empirical Parameter of Solvent Polarity [$E_T(30)$ and E_T^N]

Figure 2. solvents and Solvent Effects: An Introduction
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Under the application settings, solution chemistry is carried out in solvents, or liquids, which can have a significant impact on the characteristics of the dissolved solute species. The effect of solvents on chemical processes (equilibria, reaction rates), physical processes (absorption spectra, crystallization), and both is discussed in a brief historical perspective [20]-[21]. A solvatochromic parameter for determining the phrase

"solvent polarity" empirically is mentioned. With special focus on supercritical fluids, fluorous solvents, and room temperature ionic liquids as possible new reaction media, a taxonomy of solvents according to their chemical bonds is offered.

The possibility for tailoring DES properties through the modification of hydrogen bonding and C-H interactions is also shown by the examination of the correlations between particular interactions and thermodynamic features. This realization might open the door to creating DESs with tailored properties for certain uses, such as catalysis or separation procedures. The thorough data analysis of the study offers helpful recommendations for future research projects and offers a comprehensive framework for investigating the complex behaviors of solvent systems, advancing the development of sustainable and effective chemical processes.

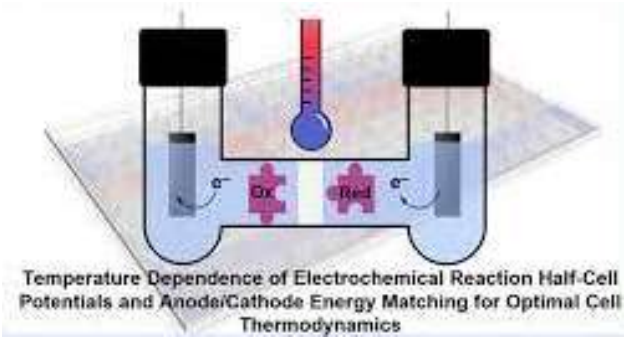

Figure 3. On the Temperature Sensitivity of Electrochemical Reaction Thermodynamics
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We describe a technique for estimating the thermodynamic potentials of electrochemical reactions at various temperatures in this article. We estimate the temperature sensitivity for a family of 27 known half reactions using a two-term Taylor series approximation of thermodynamic potential as a function of temperature. To identify the best voltage matches between cathode and anode half-cell pairings, we do additional analysis. We also address the effects of temperature variations on the voltages of the entire cell. We anticipate further interest in temperature and idealized half-reaction pairing as experimental options for the improvement of electrochemical processes based on these findings [22]-[23].

Interpretation

The significance of molecular interactions and charge transfer events in controlling the behavior of deep eutectic solvents (DESs) is highlighted by the interpretation of this study. A complete picture of DES behavior is created by fusing quantum chemical simulations with experimental results, highlighting the importance of hydrogen bonding and C-H interactions as stabilizing elements in these solvent systems . An important understanding of the connection between molecular interactions and physical properties may be gained by analyzing correlations between the sum of bond ordering of particular interactions and the melting temperatures of DESs. This view emphasizes how these interactions may be precisely controlled to change the attributes of DESs, providing a logical method for creating DESs with specific qualities.

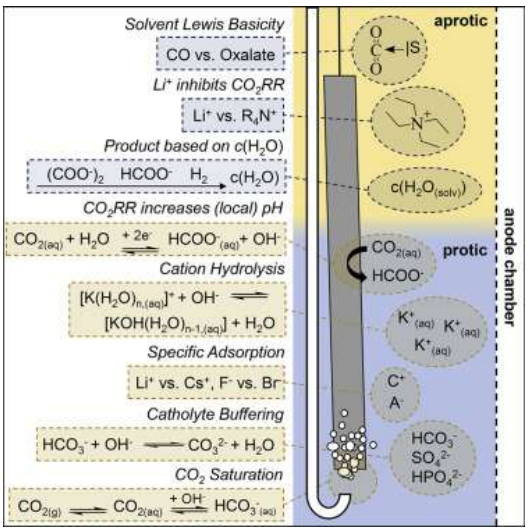

Figure 4. Solvents and Supporting Electrolytes in the Electrocatalytic Reduction of CO2
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The performance of the catalyst in the aqueous electrocatalytic CO2 reduction process (CO2RR) is significantly influenced by the electrolytes used. The local reaction conditions are affected by their concentration, species, buffer capacity, and pH value, which has an effect on the electrocatalyst's product distribution. The basicity, CO2 solubility, conductivity, and toxicity of potential solvents are significant characteristics that influence the CO2RR and the solvents' application. The effects of various electrolytes are frequently not fully understood since the complexity of an electrochemical system prevents a straightforward correlation between a single parameter and cell performance indicators like the Faradaic efficiency. A deeper comprehension of the impacts discussed in this review can aid in the construction of scalable electrolyzers and the performance prediction for an industrial application [24]-[25].

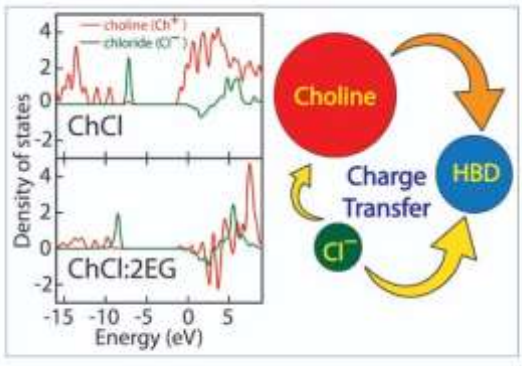

Figure 5. Quantum Chemical Insight into the Interactions and Thermodynamics Present in Choline Chloride Based Deep Eutectic Solvents
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We present the results of quantum chemical calculations on three well-known deep eutectic solvents (DESs) to clarify the molecular interactions, charge transfer interactions, and thermodynamics of these systems. The three DESs under investigation are 1:1 choline chloride/malonic acid (maloline), 1:2 choline chloride/ethylene glycol (reline), and 1:2 choline chloride/urea (ethaline) [26]-[27]. dentification of the major interactions in the DES systems was made possible by the good correlation between computed and observed vibrational spectra . It was discovered that the DESs are stabilized by both common hydrogen bonds and interactions amongst the components (C-H•••O/C-H•••). The hydrogen-bonding network established in the DES is obviously different from the plain hydrogen-bond donor dimer's hydrogen-

bonding network. Significant charge transfer from choline and chloride to the hydrogen-bond donor is shown by charge decomposition analysis, with a greater contribution from.

The interpretation also highlights the importance of combining experimental and computational data in order to have a comprehensive knowledge of DES behavior. The experimental findings from gas-liquid chromatography (GLC) measurements support the theoretical hypotheses and put the calculated results into a practical context. Indicating the consistency and dependability of the inferred results is the quantification of solute-solvent interactions, adsorption isotherms, and retention behavior by GLC. Our understanding of DES behavior is improved by this multidimensional approach, which enables a thorough investigation of charge transport .

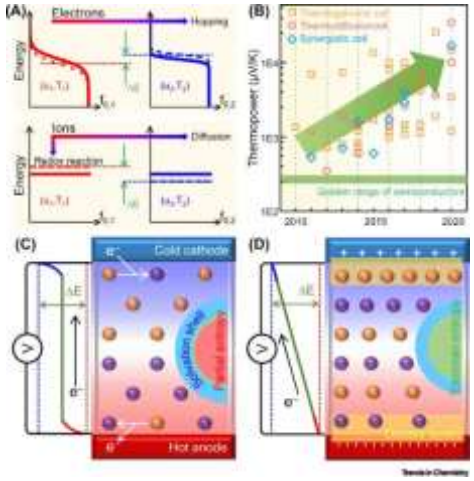

Figure 6. High-efficiency thermocells driven by thermo-electrochemical processes
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Through temperature-dependent redox processes and/or ion diffusion, thermocells, also known as thermo-electrochemical cells, are a potential technique for transforming low-grade heat (200°C) into electricity [28]-[29]. By enhancing thermo-electrochemical processes, recent advances in thermocells have included Seebeck coefficients up to 34 mVK-1 and efficiencies up to 11%. Proof-of-concept devices can generate 100 mW or more of electricity by capturing solar or ambient body heat, which are reliable energy sources for many different electronic devices. However, the quick rate of advancements in this field also sparks intense debates about issues like instability, low power density, and the deterioration of redox couples. Here, we present a comprehensive discussion on the state of engineering knowledge for enhancing thermocell performance and look at a few cutting-edge engineering techniques for.

Additionally, the interpretation draws attention to the findings' wider implications, which go beyond their direct application to DESs. The relationships between certain interactions and thermodynamic characteristics that have been found to be correlated offer a framework for comprehending solvent behavior in various systems. This knowledge can be used in many different areas, including as catalysis, separation techniques, and material synthesis .This discovery makes a significant contribution to our basic understanding of solvent systems by illuminating the complex mechanisms that control DES behavior. It also gives new perspectives that may help us develop chemical processes that are more efficient and environmentally friendly in the future [30]-[31].

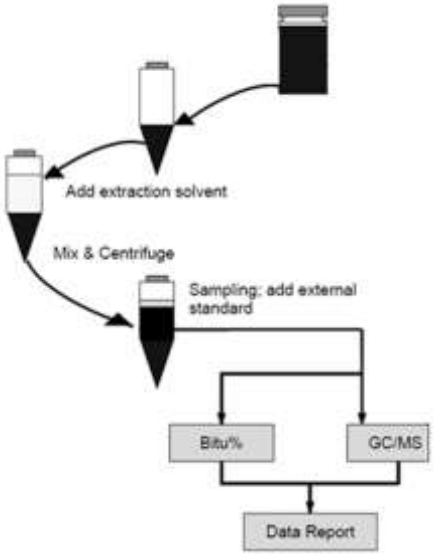

Figure 7. Thermodynamic Properties Investigation of Process Volatile Organic Compounds (VOCs) and Its Transport Impact Factor in Oil Sands Management.
https://images.app.goo.gl/JaQuqgsc6QXfSs7r8

In order to determine the characteristics of volatile organic compounds (VOCs) and the factors influencing their movement during oil sands management procedures, a novel method is presented in this study. It also explores the interaction between varying asphaltene concentration and various solvents. The discussion focuses on thermodynamics, including partitioning coefficients (Kr), specific retention volumes (Vg), activity coefficients (), and solution enthalpies (H0). Experimental measurements from gas-liquid chromatography (GLC) were used as the test data. Different asphalt concentrations (0, 2.56, 9.93, 36.86, and 53.67 wt%) have been evaluated using a variety of solvents (nC5, iC5, nC6, nC7, and toluene). Temperatures between 333.2 and 393.2 K (with a 10 K increase) were used for the experiments, respectively. Calculated are the dynamical properties of the asphalt mixture, and the relationship between .

Comparison

This study stands out as a thorough investigation of deep eutectic solvents (DESs), providing insight into their behavior through a combination of experimental and theoretical methods . This research gives a more comprehensive insight as compared to earlier studies, which frequently concentrated on particular facets of DES behavior, because it addresses molecular interactions, charge transport, and thermodynamic properties all at once. By bridging the gap between theoretical calculations and actual findings, this thorough analysis offers a greater understanding of the intricate behavior of DES systems .

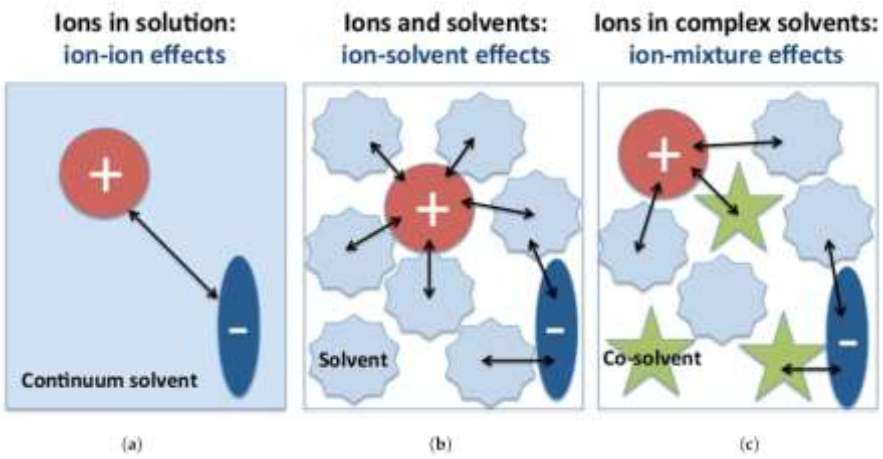

Figure 8. Properties of Ion Complexes and Their Impact on Charge Transport in Organic Solvent-Based Electrolyte Solutions for Lithium Batteries: Insights from a Theoretical Perspective
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Electrolyte formulations in typical lithium ion and lithium metal batteries are complicated combinations of numerous components. The impact of ion complexes in multicomponent electrolyte solutions on charge transport processes is discussed in this article's molecular key principles section [32]-[33]. We provide an overview of the fundamental ideas that can be utilized to explain ion-solvent and ion-ion interactions and to explain current experimental and computational findings about contemporary electrolyte formulations. As a further step toward a more in-depth comprehension of ion behavior in organic solvents, we also explore advantages and disadvantages of empirical conceptions in compared to molecular theories of solution. The conclusions of our discussion justify the advantages of ions, solvents, co-solvents, and additional compounds and point out potential directions for further developing innovative electrolyte solutions .

Furthermore, this research employs a multidimensional strategy that incorporates both approaches, in contrast to studies that are solely based on experimental observations or theoretical calculations alone . Through this special integration, theoretical predictions are validated by experimental data while molecular-level comprehension of interactions and dynamics is provided by computational insights. This blending of methods improves the accuracy and breadth of the conclusions, strengthening their robustness and their applicability to a range of applications, from catalysis to materials research .

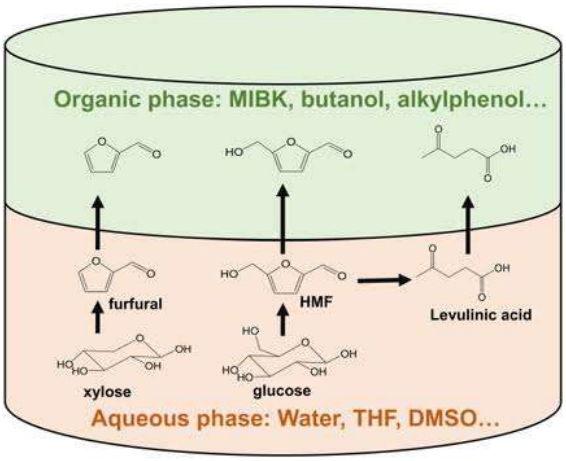

Figure 9. Organic Solvent Effects in Biomass Conversion Reactions
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The conversion of lignocellulosic biomass into fuels and chemicals has been the subject of extensive research recently. Finding suitable solvent solutions that can enhance the conversion of biomass into value-added compounds has received a lot of attention. These initiatives were made in light of a wealth of research findings that indicate organic solvents can enhance the conversion and selectivity of biomass to platform molecules [34]-[35].

We give an overview of these impacts of organic solvents that are used in biomass conversion processes, such as the generation of lignin monomers, the conversion of biomass to sugars, and the conversion of carbohydrates to furanic compounds. While discussing the causes of the problem, particular focus is made on contrasting the effects of the solvent on conversion and product selectivity in water with those in organic solvents. associated with solvent use could assist researchers in choosing and designing improved solvent systems for targeted biomass conversion processes.

This study stands out for its thorough evaluation of both elements within a single framework when compared to earlier studies that only focused on thermodynamic issues or charge transport events within DESs. The discovered relationships between particular interactions and physical characteristics provide a novel understanding of how molecular dynamics and macroscopic phenomena interact. A perspective that could direct the development of new solvents for specific applications is provided by such a thorough approach, which deepens our understanding of how certain interactions affect the overall stability and characteristics of DESs .

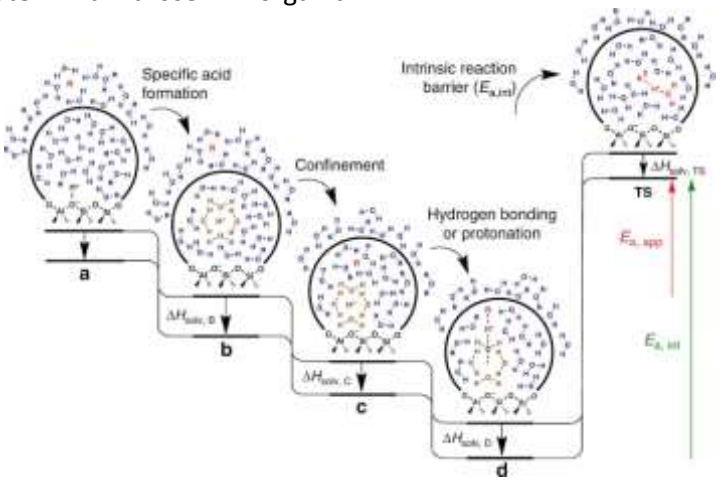

Figure 10. Understanding solvent effects on adsorption and protonation in porous catalysts
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Since there is still a dearth of predictive knowledge of the solvent effect, choosing the right solvent is a pressing difficulty in the development of effective and selective liquid phase catalytic processes [36]-[37]. In this study, an attenuated total reflection infrared spectroscopy technique is created in order to separate the thermodynamic contributions of pore-phase proton transfer from those of van der Waals interactions within zeolite pore walls when measuring the adsorption isotherms on porous materials in solvent . While the confinement (adsorption) step is significantly impacted by both the pore diameter and the solvent identity, proton-transfer is mostly affected by the solvent identity. Combining computational and experimental research reveals that water, acetonitrile, and 1,4-dioxane are the sequence in which pore-phase proton transfer to pyridine is most advantageous. We present equilibrium methods for the quantitative estimation of basic thermodynamic variables, independent of mass transfer restrictions [38]-[40].

CONCLUSION

This study concludes with a thorough investigation of deep eutectic solvents (DESs) using a coordinated strategy of experimental observations and quantum chemical computations. By analyzing the complicated chemical interactions, charge transfer events, and thermodynamic characteristics of these systems, the work provides a profound insight of DES behavior. The discovered relationships between certain interactions and physical attributes offer important clues for the

logical design of DESs with specialized properties for various applications. This research improves our understanding of solvent behavior by bridging the gap between theoretical predictions and actual data. It also provides a comprehensive foundation for enhancing DES performance and application across numerous disciplines.

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