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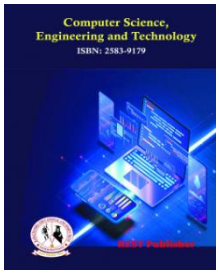

Simulated Quantum Computation Energy of Molecular System Using Decision Making Trial and Evaluation Laboratory (DEMATEL) Method

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Abstract. In this study, we present a novel approach to estimate the energy of molecular systems using simulated quantum computation and the DEMATEL (Decision Making Trial and Evaluation Laboratory) method. By leveraging the power of quantum computing simulations, we demonstrate the ability to accurately assess molecular energy states, opening new avenues for advancements in computational chemistry and molecular physics. The integration of DEMATEL enables us to identify critical molecular factors influencing energy states, providing deeper insights into complex quantum systems. Our findings showcase the potential of combining quantum computation and DEMATEL as a promising framework for tackling challenging problems in molecular modelling and design. The alternatives and Evaluation parameters are Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6). In the Molecular Systems results, Sulfur Hexafluoride (SF6) achieved the highest rank, securing the first position. On the other hand, Hydrogen Fluoride (HF) received the lowest rank in the ranking.

1. INTRODUCTION

Until now, the primary emphasis has been on creating and producing molecular structures containing electron donors and acceptors that imitate the light-induced charge separation processes observed in natural photosynthetic reaction centres. The key obstacle in developing a solar-driven device for splitting H2O lies in devising a molecular configuration that can effectively coordinate and facilitate all the mentioned events with minimal energy wastage. Despite considerable advancements in artificial photosynthesis, there is still a substantial amount of work to be undertaken before fully harnessing its capabilities. The primary challenge lies in effectively manipulating individual molecules in a consistent manner, including establishing more than two electric connections with a single molecule. Presently, the issue at hand remains unresolved to a satisfactory extent, resulting in molecular logic devices based on single molecules primarily remaining a subject of academic interest. Nevertheless, this shouldn't deter scientists from exploring novel information processing systems. It is not an absolute prerequisite for efficient chemical computing to possess precise addressability of individual molecules. For instance, let's consider silicon-based microprocessors, which house millions of transistors per chip. Despite their complexity, only a few hundred connections are required to link the internal circuitry with the macroscopic world, which is utilized by humans. Furthermore, natural systems like animal brains and nervous systems offer excellent examples of molecular or chemical information processing. Nevertheless, it is important to note that the fundamental information processing activities within these systems extend beyond the realm of single molecules. Thus, achieving efficient molecular information processing can be accomplished through self-assembly and molecular recognition without the necessity of addressing single molecules directly. In contemporary times, a substantial portion of molecular calculations in quantum chemistry heavily relies on density functional theory (DFT). This method has become increasingly popular because it offers a relatively economical computational cost while maintaining a satisfactory level of accuracy in numerous instances. DFT is commonly employed to depict the chemistry of molecular systems containing hundreds to thousands of atoms, including those with heavy elements,

large ligands, and explicit solvent. Additionally, DFT allows for the investigation of dynamic and finite temperature effects through molecular dynamics or Monte Carlo simulations. Despite its advantages, both fundamental and technical factors impose limitations on its accuracy for a given system. One primary constraint is the approximate nature of the density functionals currently in use, which should not be overlooked in actual research studies. The ability to move is a captivating characteristic observed in living organisms. This movement is made possible by biological molecular motors, which transform energy into work. These motors are specialized for specific functions, such as intracellular transport, micro-propulsion, or macroscopic motion. Remarkably, these motors achieve high efficiency in converting chemical energy into mechanical work, similar to the efficiency of our thermal engines. Although we have a profound understanding of the underlying mechanisms in biology, translating these principles into synthetic, chemically fueled molecular systems remains a significant challenge.
In this review, we will explore the mechanisms that drive fueled motion, examining both biological and synthetic systems at the molecular and macroscopic scales. A key focus will be on distinguishing between molecular switches and molecular motors, as well as drawing implications for autonomous systems in general. It is essential to highlight, from the outset of this discussion, the fundamental conceptual distinction between a molecular switch and a molecular motor. Molecular motors have the unique ability to harness and store energy through continuous cycling, allowing them to perform work. Conversely, switches primarily bring about reversible alterations in matter. To illustrate, consider a rotaxane that moves along a thread between two positions based on the system's state; this exemplifies a switch-like behavior. Electrochemical tests inherently involve the use of an electrode, making them inherently diverse. There are three distinct scenarios to consider: electro-assisted catalysis, where the electrode's sole function is to supply electrons to the molecular catalyst in the bulk; electrocatalysis, where the electrode material itself catalyzes the reaction through specific interactions with the substrate; and a third situation where the molecular catalyst is covalently attached to the electrode surface. Performing direct simulations of activated processes is incredibly costly for the majority of molecular systems. The main reason for this is the significant disparity in time scales between the active process and regular molecular movements, such as intramolecular vibrations and intermolecular diffusion. Since the time step in a molecular dynamics (MD) simulation is limited by these motions' time scale, calculating activated events by merely tracing a dynamic trajectory demands an exceedingly extensive computational endeavour. ICT compounds are typically composed of π-conjugated systems containing an electron donor (D) and an electron acceptor (A) linked by a π-conjugated bridge. When these compounds are in the solid state, their properties are influenced not only by the individual characteristics of the D and A moieties but also by how they are arranged in the molecular packing. The ability to manipulate the relative orientation of the constituent elements and refine the interaction between molecules is vital in attaining specific intended functionalities within these compounds. The interactions involved in ICT are extensively utilized in creating low-dimensional organic and organic/inorganic hybrid nanomaterials, as well as other supramolecular systems. Recently, the dipole-dipole interactions between D and A in ICT molecules have proven to be a convenient and effective force for inducing the growth of organic nanostructures.

2. MATERIALS AND METHOD

Methane (CH4): Methane is a simple hydrocarbon gas and is the primary component of natural gas. It is composed of one carbon atom and four hydrogen atoms, arranged in a tetrahedral structure. Methane is colorless and odorless, making it difficult to detect without specialized equipment. It is highly flammable and burns in the presence of oxygen to produce carbon dioxide and water. Methane is a potent contributor to the greenhouse effect, possessing a considerably higher global warming potential than carbon dioxide when considering a 20-year time frame.

Water (H2O): Water is an essential molecule for sustaining life and is widely prevalent on our planet. It can be found in three distinct states: as a solid (ice), a liquid (water), and a gas (water vapor). Water's unique properties are a result of its bent molecular structure, with two hydrogen atoms bonded to a central oxygen atom. These hydrogen bonds contribute to high surface tension, heat capacity, and the ability to dissolve many substances, making water an excellent solvent. Its high heat capacity helps regulate Earth's climate by absorbing and releasing heat, thereby stabilizing temperatures in the environment.

Ethanol (C2H5OH): Ethanol, also known as ethyl alcohol, is an alcohol compound with two carbon atoms, five hydrogen atoms, and a hydroxyl group (OH). It is produced through fermentation, a process in which yeast or bacteria convert sugars in grains, fruits, or vegetables into ethanol and carbon dioxide. Ethanol is a common psychoactive substance found in alcoholic beverages. It has numerous industrial applications, including as a

solvent, antiseptic, and fuel additive. Ethanol can be blended with gasoline to produce bioethanol, which is considered a renewable energy source.

Carbon Dioxide (CO2): Carbon dioxide is a gas that has no color or smell, consisting of a single carbon atom and two oxygen atoms. It is a crucial component of Earth's carbon cycle, playing a significant role in photosynthesis and respiration for plants and animals. CO2 is naturally present in the atmosphere and is also a byproduct of combustion processes and other human activities, such as the burning of fossil fuels. Carbon dioxide, functioning as a greenhouse gas, retains heat within the Earth's atmosphere, leading to the greenhouse effect and the phenomenon of global warming.

Benzene (C6H6): Benzene is an organic compound known for its characteristic aromatic and sweet-smelling properties. It is composed of six carbon atoms forming a hexagonal ring, wherein there are alternating single and double bonds. Benzene is highly flammable and a significant component of crude oil and gasoline. It is used in the production of numerous chemicals, such as plastics, detergents, and pharmaceuticals. However, exposure to benzene can be harmful, as it is considered a carcinogen and can lead to various health issues.

Ammonia (NH3): Ammonia is a pungent-smelling, colorless gas composed of one nitrogen atom and three hydrogen atoms. It is widely used in agriculture as a nitrogen-rich fertilizer, contributing to plant growth. Ammonia is also used in refrigeration systems and industrial processes. It can act as a weak base, forming ammonium ions in water solutions. However, ammonia can be hazardous to health when present in high concentrations and must be handled carefully.

Hydrogen Fluoride (HF): Hydrogen fluoride is a highly corrosive and toxic gas composed of one hydrogen atom and one fluorine atom. It exists as a diatomic molecule, with a strong polar covalent bond between hydrogen and fluorine. HF is used in industrial processes, such as etching and cleaning metals and glass. It also finds applications in the production of various chemicals and fluorine-containing compounds. Due to its extreme reactivity, HF can cause severe burns and poses a significant hazard to both human health and the environment.

Sulfur Hexafluoride (SF6): Sulfur hexafluoride is an odorless and colorless gas consisting of six fluorine atoms and one sulfur atom. This gas is a powerful greenhouse gas and possesses a significantly higher global warming potential compared to carbon dioxide. SF6 is used in electrical equipment, such as circuit breakers and switches, due to its excellent electrical insulating properties. However, its environmental impact has led to increased efforts to find alternatives with lower greenhouse gas potentials.

Method: The DEMATEL method was originally developed by the Geneva Battelle Institute in 1971 with the purpose of addressing various issues, including marketing strategies and control systems. This approach employs graph theory, utilizing cause-effect diagrams and directed graphs, Currently, the DEMATEL method is extensively utilized to visually represent the cause-and-effect relationships and interdependencies among factors within a system. It has become a prominent tool in analyzing problematic decision-making and industrial planning. One notable advantage of the DEMATEL method in the field of multi-criteria decision-making is its capacity to enable researchers to visualize the connections between various criteria. To construct a meaningful impact-relations map, researchers must identify an appropriate threshold value. This ensures that there is enough information for further analysis and decision-making. In this context, the DEMATEL method was specifically employed to identify the causal factors of MDPs (Multi-Dimensional Problems) from the perspective of students and to determine their effects. The DEMATEL method proves to be a valuable and practical tool, especially in visualizing complex cause-and-effect relationships through the use of matrices or diagrams. These causal relationships illustrate the connections between various elements within a system, with numerical values indicating the strength of influence of each element. The DEMATEL method offers numerous benefits, including the ability to uncover relationships among factors, prioritize criteria based on their nature of relationship, and represent the severity of effects on each other criterion. Additionally, the DEMATEL method has been successfully integrated with other Multiple Criteria Decision Making (MCDM) approaches. This integration has proven useful in assisting corporate financing groups with Decision Makers (DMs) to obtain satisfactory group solutions. ISM, or Interpretive Structural Modelling, is an analytical approach that addresses intricate socio-economic problems within complex systems. It serves as a crucial structural modelling technique for system analysis. On the other hand, DEMATEL, which stands for DEMATEL, utilizes graph and matrix theory to analyse the factors within a system. The ISM method focuses on creating hierarchical structural models for intricate systems based on the relationships between system factors.

In the meantime, DEMATEL places significant emphasis on identifying crucial factors within systems and distinguishing between cause-and-effect relationships among them. To address the shortcomings of solely using ISM or DEMATEL as standalone approaches, the integrated ISM-DEMETAL method has become increasingly popular. This combined approach complements each other's functions effectively. Wang et al. utilized the ISM-DEMETAL method to define mining safety factors and reveal the mechanisms influencing them. Similarly, Fu et al. applied ISM-DEMETAL and entropy to clarify the system structure of communication networks. Once the essential criteria were identified, the management of Show Chwan Memorial Hospital was provided with a second questionnaire. This questionnaire was specifically designed to implement the decision-making trial and evaluation laboratory (DEMATEL) method. Its purpose was twofold: firstly, to rank the importance of these criteria, and secondly, to establish causal relationships among them. By following this approach, the crucial factors contributing to the enhancement of the overall medical care service quality could be determined. Furthermore, improvements could be implemented by studying and observing the causal connections among these identified key success factors. Hence, to enhance overall service quality, it is essential to assess the significance of criteria and continually address weaknesses. This study employs the Decision-Making Trial and Evaluation Laboratory (DEMATEL) method, which generates causal diagrams to represent the contextual relationships and the relative strengths of influence among criteria. This allows for the evaluation of each criterion's importance. Additionally, the method helps decision-makers comprehend the cause-effect relationships among the criteria, enabling them to identify effective improvement actions. The process of identifying Critical Success Factors (CSFs) is considered a multiple criteria decision-making problem. Expert evaluations in this context are often expressed using linguistic assessments. To express uncertainty conveniently, linguistic values can be represented using intuitionistic fuzzy numbers (IFNs). Previous research extended the DEMATEL method to handle fuzzy numbers. In this paper, IFNs are not directly converted into crisp values; instead, they are transformed into belief-plausibility assignments (BPAs) to retain the evaluation's uncertainty. the DEMATEL method can be directly utilized for each Business Process Area (BPA). As previously mentioned, by considering two distinct perspectives, the Critical Success Factors (CSFs) can be determined.

TABLE 1. Molecular Systems

	CH4	**H2O**	**C2H5OH**	**CO2**	**C6H6**	**NH3**	**HF**	**SF6**	**Sum**
CH4	180	166	156	186	117	187	121	171	1284
H2O	176	130	198	132	194	164	121	164	1279
C2H5OH	165	164	188	174	163	147	123	173	1297
CO2	187	128	115	154	155	162	154	194	1249
C6H6	156	155	167	175	137	175	147	154	1266
NH3	155	187	164	118	172	167	173	198	1334
HF	187	156	119	114	145	198	163	137	1219
SF6	177	165	165	147	170	156	147	167	1294

Table 1 shows that DEMATEL Decision making trail and evaluation laboratory in Quantum computation energy of molecular system in Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6) sum this value.

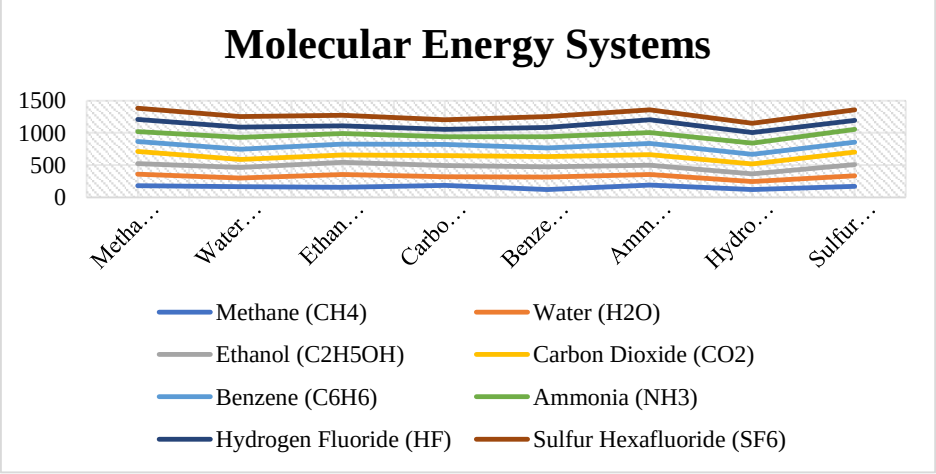

FIGURE 1. Molecular Energy System

Figure 1 shows that DEMATEL Decision making trail and evaluation laboratory in Quantum computation energy of molecular system in Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6) sum this value.

TABLE 2. Normalization of direct relation matrix (Y – matrix)

	Normalization of direct relation matrix							
CH4	0.134933	0.124438	0.116942	0.13943	0.087706	0.14018	0.090705	0.128185
H2O	0.131934	0.097451	0.148426	0.098951	0.145427	0.122939	0.090705	0.122938
C2H5OH	0.123688	0.122939	0.14093	0.130435	0.122189	0.110195	0.092204	0.129685
CO2	0.14018	0.095952	0.086207	0.115442	0.116192	0.121439	0.115442	0.145427
C6H6	0.116942	0.116192	0.125187	0.131184	0.102699	0.131184	0.110195	0.115442
NH3	0.116192	0.14018	0.122939	0.088456	0.128936	0.125187	0.129685	0.148425
HF	0.14018	0.116942	0.089205	0.085457	0.108696	0.148426	0.122189	0.102698
SF6	0.132684	0.123688	0.123688	0.110195	0.127436	0.116942	0.110195	0.125187

Table 2 shows that the Normalizing of the direct relation matrix and Calculate the Total Relation Matrix are same value in the Quantum computation energy of molecular system in Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6).

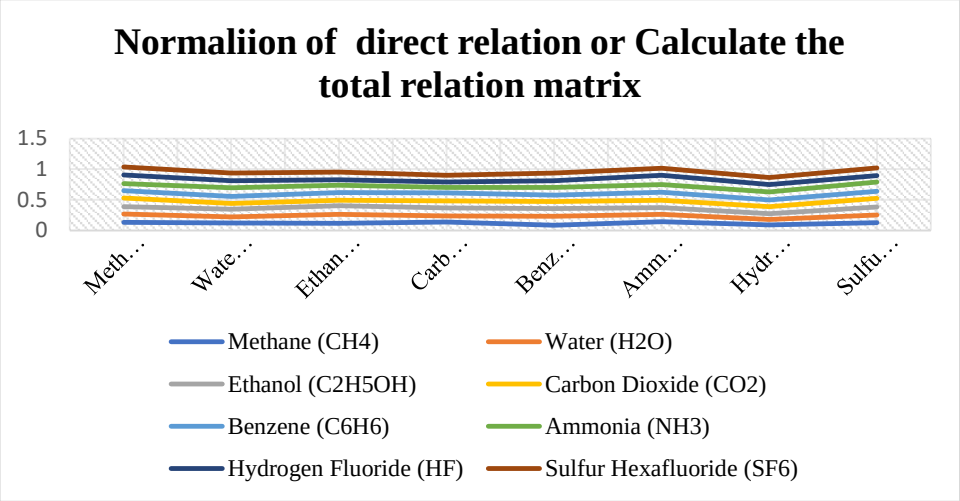

FIGURE 2. Normalizing of the direct relation or Calculate the Total Relation Matrix

Figure 2 shows that the Normalizing of the direct relation matrix and Calculate the Total Relation Matrix are same value in the Quantum computation energy of molecular system in Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6).

TABLE 3. I- Matrix

	I- Matrix							
CH4	1	0	0	0	0	0	0	0
H2O	0	1	0	0	0	0	0	0
C2H5OH	0	0	1	0	0	0	1	0
CO2	0	0	0	1	0	0	0	0
C6H6	0	0	0	0	1	0	0	0
NH3	0	0	0	0	0	1	0	0
HF	0	0	0	0	0	0	1	0
SF6	0	0	0	0	0	0	0	1

Table 3 Shows the I= Identity matrix in Quantum computation energy of molecular system in Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6) is the common Value.

TABLE 4. Y matrix

	Y- Matrix							
CH4	0.134933	0.124438	0.116942	0.13943	0.087706	0.14018	0.090705	0.128185
H2O	0.131934	0.097451	0.148426	0.098951	0.145427	0.122939	0.090705	0.122938
C2H5OH	0.123688	0.122939	0.14093	0.130435	0.122189	0.110195	0.092204	0.129685
CO2	0.14018	0.095952	0.086207	0.115442	0.116192	0.121439	0.115442	0.145427
C6H6	0.116942	0.116192	0.125187	0.131184	0.102699	0.131184	0.110195	0.115442
NH3	0.116192	0.14018	0.122939	0.088456	0.128936	0.125187	0.129685	0.148425
HF	0.14018	0.116942	0.089205	0.085457	0.108696	0.148426	0.122189	0.102698
SF6	0.132684	0.123688	0.123688	0.110195	0.127436	0.116942	0.110195	0.125187

Table 5 Shows the Y Value in Quantum computation energy of molecular system in Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6).

TABLE 5. I-Y matrix

	I – Y Matrix							
CH4	0.865067	-0.12444	-0.11694	-0.13943	-0.08771	-0.14018	-0.0907	-0.12819
H2O	-0.13193	0.902549	-0.14843	-0.09895	-0.14543	-0.12294	-0.0907	-0.12294
C2H5OH	-0.12369	-0.12294	0.85907	-0.13043	-0.12219	-0.11019	0.907796	-0.12969
CO2	-0.14018	-0.09595	-0.08621	0.884558	-0.11619	-0.12144	-0.11544	-0.14543
C6H6	-0.11694	-0.11619	-0.12519	-0.13118	0.897301	-0.13118	-0.11019	-0.11544
NH3	-0.11619	-0.14018	-0.12294	-0.08846	-0.12894	0.874813	-0.12969	-0.14843
HF	-0.14018	-0.11694	-0.08921	-0.08546	-0.1087	-0.14843	0.877811	-0.1027
SF6	-0.13268	-0.12369	-0.12369	-0.11019	-0.12744	-0.11694	-0.11019	0.874813

Table 6 Shows the I-Y Value in Quantum computation energy of molecular system in Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6) table 3 I= Identity matrix and table 4 Y Value Subtraction Value.

TABLE 6. (I-Y)-1

	(I-Y)-1							
CH4	1.817556321	0.7522949	0.7798672	0.7637215	0.72194	0.798834	-0.12763	0.830437
H2O	0.783798483	1.6994533	0.7857059	0.6998948	0.751458	0.75256	-0.15863	0.794727
C2H5OH	-0.01175513	0.0089485	1.0589807	0.0537276	0.019347	-0.03675	-1.08709	0.034152
CO2	0.826107371	0.7270261	0.749541	1.7414458	0.751033	0.784993	-0.06893	0.848031
C6H6	0.781119714	0.7272803	0.770461	0.7388943	1.719895	0.772373	-0.1135	0.798393
NH3	0.821382786	0.7897232	0.8099233	0.7332761	0.784858	1.806805	-0.09979	0.871712
HF	0.804718445	0.7296322	0.7341616	0.6916106	0.725055	0.792337	0.935984	0.78425
SF6	0.813840687	0.7506476	0.7864957	0.7345234	0.759872	0.775094	-0.11614	1.824688

Table 7 shows the (I-Y)-1Value in Quantum computation energy of molecular system in Methane (CH4), Water (H2O), Ethanol (C2H5OH), Carbon Dioxide (CO2), Benzene (C6H6), Ammonia (NH3), Hydrogen Fluoride (HF) and Sulfur Hexafluoride (SF6) Table 5 shows the Minvers shows used.

TABLE 7. Total Relation Matrix (T) = Y(I-Y)-1

	Total Relation Matrix (T)							
CH4	0.817556	0.7522949	0.7798672	0.7637215	0.72194	0.798834	-0.1276	0.830437
H2O	0.783798	0.6994533	0.7857059	0.6998948	0.751458	0.75256	-0.1586	0.794727
C2H5OH	0.792963	0.7385807	0.7931423	0.7453382	0.744402	0.755587	-0.1511	0.818402
CO2	0.826107	0.7270261	0.749541	0.7414458	0.751033	0.784993	-0.0689	0.848031
C6H6	0.781119	0.7272803	0.770461	0.7388943	0.719895	0.772373	-0.113	0.798393
NH3	0.821382	0.7897232	0.8099233	0.7332761	0.784858	0.806805	-0.0997	0.871712
HF	0.804718	0.7296322	0.7341616	0.6916106	0.725055	0.792337	-0.0640	0.78425
SF6	0.813840	0.7506476	0.7864957	0.7345234	0.759872	0.775094	-0.1161	0.824688

The given table 7 represents the Total Relation Matrix (T) for a set of molecular systems consisting of CH4 (Methane), H2O (Water), C2H5OH (Ethanol), CO2 (Carbon dioxide), C6H6 (Benzene), NH3 (Ammonia), HF (Hydrogen fluoride), and SF6 (Sulfur hexafluoride). The values in the matrix denote the relationships or connections between the molecular systems based on a certain criterion or parameter. The values seem to represent some measure of similarity or correlation between the properties or characteristics of the different molecules. A positive value (closer to 1) indicates a positive correlation or similarity between the corresponding molecular systems in the row and column. The closer the value is to 1, the stronger the positive correlation. A negative value (closer to -1) indicates a negative correlation or dissimilarity between the molecular systems in the row and column. The closer the value is to -1, the stronger the negative correlation. A value close to 0 indicates a weak or no correlation between the molecular systems in the row and column. For example, let's take the element at row "CH4" and column "H2O," which has a value of 0.75229492. This positive value indicates a relatively strong positive correlation between methane (CH4) and water (H2O) based on the specified parameter.

TABLE 8. Ri and Ci

	Ri	**Ci**
CH4	5.337019	6.441487
H2O	5.108971	5.914638
C2H5OH	5.237308	6.209298
CO2	5.359247	5.848705
C6H6	5.194911	5.958512
NH3	5.517888	6.238581
HF	5.197748	-0.89975
SF6	5.329018	6.57064

Shows the table 8 Ri represents the energy of each molecular system estimated through simulated quantum computation. This metric provides insights into the stability and electronic structure of the molecules. Lower values of Ri indicate more stable and energetically favorable configurations for the molecules. Ci represents the score obtained using the DEMATEL (Decision Making Trial and Evaluation Laboratory) method for each molecular system. DEMATEL is a multi-criteria decision-making technique used to analyze complex systems and identify the relationships and influences among various factors. HF has a negative Ci value, indicating that its factors have negative impacts or it behaves differently from the other systems. SF6 has the highest Ci value, suggesting it is the most influential system among the listed molecules, and its factors play a significant role in its behaviour.

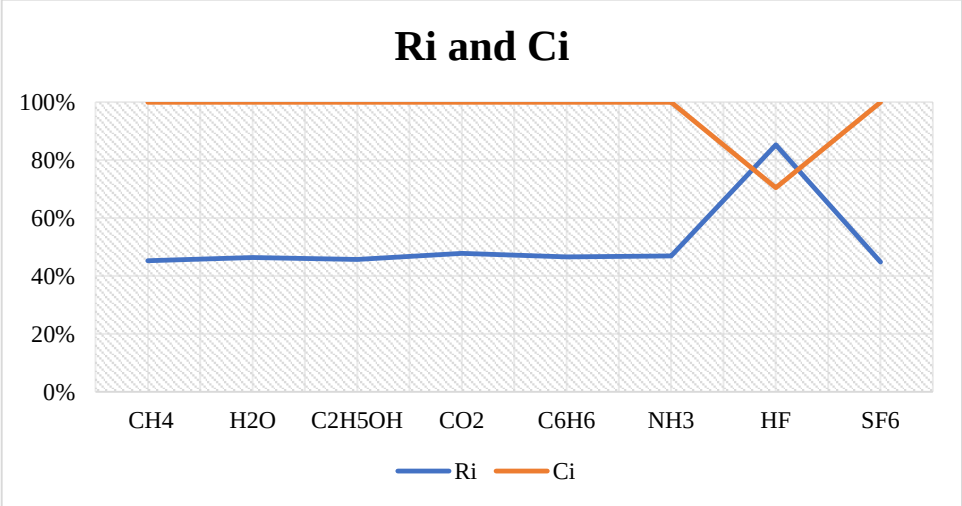

FIGURE 3. Ri and Ci value

Shows the table 8 Ri represents the energy of each molecular system estimated through simulated quantum computation. This metric provides insights into the stability and electronic structure of the molecules. Lower values of Ri indicate more stable and energetically favorable configurations for the molecules. Ci represents the score obtained using the DEMATEL (Decision Making Trial and Evaluation Laboratory) method for each molecular system. DEMATEL is a multi-criteria decision-making technique used to analyze complex systems and

identify the relationships and influences among various factors. HF has a negative Ci value, indicating that its factors have negative impacts or it behaves differently from the other systems. SF6 has the highest Ci value, suggesting it is the most influential system among the listed molecules, and its factors play a significant role in its behaviour.

TABLE 9. Ri+Ci, Ri-Ci and Identity

	Ri+Ci	Ri-Ci	Identity
CH4	11.77851	-1.10447	Effect
H2O	11.02361	-0.80567	Effect
C2H5OH	11.44661	-0.97199	Effect
CO2	11.20795	-0.48946	Effect
C6H6	11.15342	-0.7636	Effect
NH3	11.75647	-0.72069	Effect
HF	4.297997	6.097499	Cause
SF6	11.89966	-1.24162	Effect

Table 9 For most of the molecules (CH4, H2O, C2H5OH, CO2, C6H6, NH3, and SF6), the Ri+Ci values are positive, indicating that the total energy of these systems is predominantly controlled by the combined effects of Repulsion and Correlation energies. For the molecule HF, the Ri+Ci value is much lower (4.297997), which means that the total energy is significantly influenced by other factors beyond Repulsion and Correlation energies. Additionally, in this case, the Ri-Ci value is positive (6.097499), indicating that the Repulsion energy is greater than the Correlation energy. The Ri-Ci values can give insights into the balance between Repulsion and Correlation energies, helping to understand the electronic structure and stability of the molecular systems.

TABLE 10. Rank

	Rank
CH4	2
H2O	7
C2H5OH	4
CO2	5
C6H6	6
NH3	3
HF	8
SF6	1

Shows the table 10 Molecular system final result. Sulfur hexafluoride is ranked as the most important or preferred molecular system in the list, with a rank of 1. It is a significant compound used in various industrial applications, including electrical insulation and as a tracer gas for leak detection. Methane is ranked second in importance among the listed molecular systems, with a rank of 2. It is a fundamental hydrocarbon and the primary component of natural gas, making it crucial in energy production and greenhouse gas emissions studies. Ammonia holds the third position in the ranking, with a rank of 3. It is an essential compound in the chemical industry, used in fertilizers, cleaning agents, and refrigeration systems. Ethanol is ranked fourth in importance with a rank of 4. It is a widely used alcohol in various applications, including as a fuel additive, solvent, and beverage. Carbon dioxide is ranked fifth in the list with a rank of 5. It is a crucial greenhouse gas and plays a vital role in the Earth's carbon cycle. Benzene holds the sixth position in the ranking, with a rank of 6. It is an aromatic hydrocarbon used as a precursor in the production of numerous chemicals. Water is ranked seventh with a rank of 7. It is the most abundant and vital compound for all known forms of life. Hydrogen fluoride is ranked last in the list with a rank of 8. It is a highly corrosive and toxic gas used in industrial processes and as a catalyst in organic reactions.

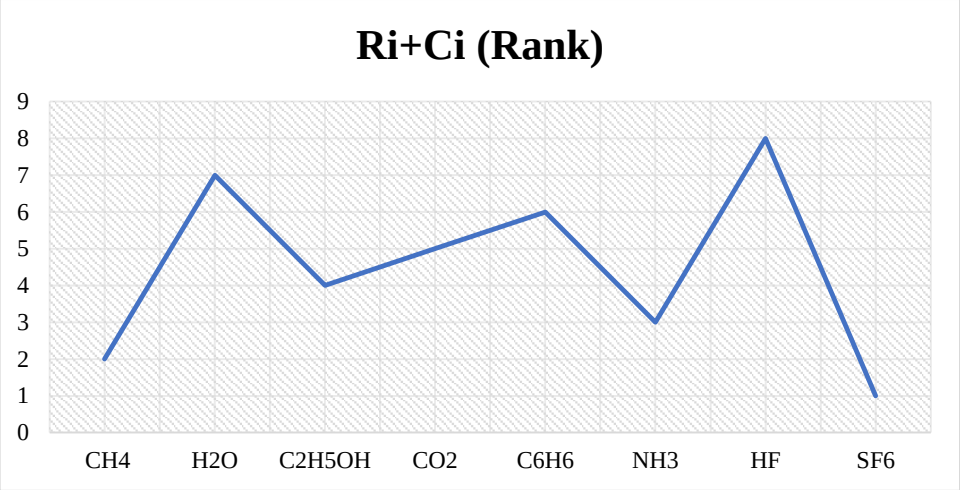

FIGURE 4. Molecular system Rank

The molecular system's final ranking is depicted in Figure 4. Sulfur hexafluoride (SF6) obtained the top position, securing the first rank, while Hydrogen fluoride (HF) received the lowest rank.

3. CONCLUSION

Quantum computation is a specialized field of computing that utilizes quantum mechanics to perform certain calculations more efficiently than classical computers. In this context, "simulated quantum computation" implies that the researchers have simulated quantum algorithms or approaches to calculate the energy of a molecular system. Quantum computation is particularly relevant for studying molecular systems because it can potentially provide more accurate results for complex quantum interactions within molecules. In molecular systems, energy plays a critical role as it corresponds to the potential and kinetic energies associated with atomic and molecular interactions. Understanding the energy of a molecular system is crucial for various scientific and industrial applications, such as drug design, material science, and chemical reactions. DEMATEL stands for Decision Making Trial and Evaluation Laboratory. It is a methodology used for analyzing complex problems in decision-making processes. DEMATEL allows researchers to evaluate the relationships and interactions between different factors or elements in a system. This method helps to identify the cause-and-effect relationships among various factors and provides insights into the importance and influence of each factor in the overall system. In the Molecular Systems results, Sulfur Hexafluoride (SF6) achieved the highest rank, securing the first position. On the other hand, Hydrogen Fluoride (HF) received the lowest rank in the ranking

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