

**“TIQXMMI” MTU HUZURIDAGI FUNDAMENTAL VA AMALIY
TADQIQOTLAR INSTITUTI HUZURIDAGI
ILMIY DARAJALAR BERUVCHI
DSc.03/06.11.2025.K/FM.10.09 RAQAMLI ILMIY KENGASH**

FUNDAMENTAL VA AMALIY TADQIQOTLAR INSTITUTI

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**IMIDAZOL HOSILALARI ASOSIDAGI ION SUYUQLIKLARDA CO₂, H₂S
VA CH₄ GAZLARINING YUTILISHINI MOLEKULYAR DINAMIKA
USULLARI YORDAMIDA TADQIQ QILISH**

02.00.04-Fizik kimyo

**FIZIKA-MATEMATIKA FANLARI BO‘YICHA FALSAFA DOKTORI (PhD)
DISSERTATSIYASI AVTOREFERATI**

Toshkent 2026

**Fizika-matematika fanlari Falsafa doktori (PhD) dissertatsiyasining
avtoreferati mundarijasi**

Contents of dissertation abstract of doctor of philosophy (PhD)

Оглавление автореферата диссертации доктора философии (PhD)

Kodirov Akbar Ismoil ugli

Molecular dynamics study of CO₂, H₂S, and CH₄ gas absorption in imidazole-based ionic liquids.....3

Qodirov Akbar Ismoil og‘li

Imidazol hosilalari asosidagi ion suyuqliklarda CO₂, H₂S va CH₄ gazlarining yutilishini molekulyar dinamika usullari yordamida tadqiq qilish 21

Қодиров Акбар Исмоил ўғли

Исследование абсорбции газов CO₂, H₂S и CH₄ в ионных жидкостях на основе производных имидазола методами молекулярной динамики 39

E‘lon qilingan ilmiy ishlar ro‘yxati

List of published works

Список опубликованных работ 43

**SCIENTIFIC COUNCIL ON AWARDING OF SCIENTIFIC DEGREE
DSc.03/06.11.2025.K/FM.10.09 AT INSTITUTE OF
FUNDAMENTAL AND APPLIED RESEARCH**

INSTITUTE OF FUNDAMENTAL AND APPLIED RESEARCH

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**MOLECULAR DYNAMICS STUDY OF CO₂, H₂S, AND CH₄ GAS
ABSORPTION IN IMIDAZOLE-BASED IONIC LIQUIDS**

02.00.04 - Physical Chemistry

**DISSERTATION ABSTRACT FOR THE DOCTOR OF PHILOSOPHY (PhD)
PHYSICAL AND MATHEMATICAL SCIENCES**

Tashkent 2026

The theme of dissertation of the doctor of philosophy (PhD) in Physical and Mathematical Sciences was registered by Supreme Attestation Commission at the Ministry of Higher Education, Science and Innovation of the Republic of Uzbekistan under B2026.2.PhD/FM1550

The dissertation was carried out at the Fundamental and Applied Research Institute under the National Research University "TIAME".

The abstract of the dissertation is posted in three languages (english, uzbek, russian (resume)) on the scientific website page of the scientific Council website (www.ifar.uz) and on the information of "Ziyonet" Information and educational portal (www.ziyonet.uz).

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The Abstract of the dissertation was distributed on "____" _____, 2026.

(Registry record № ____ dated "____" _____, 2026).

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INTRODUCTION (Annotation of PhD dissertation)

Relevance and necessity of the topic. Natural gas processing, acid-gas separation, and the development of energy-efficient gas-purification technologies are among the important scientific and practical areas worldwide. Carbon dioxide (CO_2) and hydrogen sulfide (H_2S) present in natural gas reduce its calorific value, intensify corrosion in pipelines and process equipment, and pose serious environmental and technical safety risks. At the same time, methane (CH_4) is the principal valuable component of natural gas, and preserving it as much as possible during purification is of major economic importance. Therefore, the development of efficient, stable, and regenerable absorbents for the selective separation of CO_2 and H_2S from CH_4 is an urgent task.

At present, aqueous amine solutions, physical solvents, membranes, and adsorbents are used for CO_2 and H_2S removal. However, these approaches have limitations associated with regeneration energy, corrosion, solvent loss, selectivity, and stability. Consequently, ionic liquids with low volatility, high chemical stability, and easy regeneration are considered promising alternative absorbents. In particular, imidazolium ionic liquids containing SCN^- and DCA^- anions can interact selectively with CO_2 and H_2S . Nevertheless, the absorption and molecular transport of CO_2 , H_2S , and CH_4 in $[\text{EMIM}][\text{SCN}]$, $[\text{EMIM}][\text{DCA}]$, $[\text{BMIM}][\text{SCN}]$, and $[\text{BMIM}][\text{DCA}]$ have not been sufficiently investigated comparatively within a unified computational methodology.

Considerable attention is being paid worldwide to experimental and computational studies of gas solubility, diffusion, and molecular interactions in ionic liquids. Molecular dynamics simulations, umbrella sampling, free-energy profiles, radial distribution functions, and molecular diffusion coefficients make it possible to evaluate the behavior of gas molecules at ionic-liquid interfaces and in the bulk phase at the atomic level. These approaches reveal molecular mechanisms that are difficult to observe directly in experiments, clarify the roles of gas-anion and gas-cation interactions, and explain the selectivity of absorbents.

In recent years, important studies have also been conducted in Uzbekistan on molecular modeling, atomistic analysis of physicochemical processes, and transport phenomena at gas-liquid interfaces. The development of molecular dynamics, free-energy calculations, diffusion analysis, and structural analysis provides a fundamental scientific basis for natural-gas purification, environmental safety, energy efficiency, and the development of new functional materials. From this perspective, the molecular dynamics investigation of CO_2 , H_2S , and CH_4 absorption in cyano-functionalized imidazolium ionic liquids has substantial scientific and practical significance for evaluating new absorbents for natural-gas purification.

This dissertation research contributes, to a certain extent, to the implementation of the tasks defined in Decree No. PF-60 of the President of the Republic of Uzbekistan dated 28 January 2022, “On the Development Strategy of New Uzbekistan for 2022-2026,” Resolution No. PQ-4805 of the President of the

Republic of Uzbekistan dated 12 August 2020, “On Measures to Improve the Quality of Continuous Education and the Effectiveness of Science in the Fields of Chemistry and Biology,” and other regulatory documents related to this field.

Conformity of the research to the main priorities of science and technology development of the republic. This research was carried out in accordance with Priority Direction VII, “Chemical Technologies and Nanotechnologies,” of the Republic’s science and technology development priorities.

Degree of problem investigation. Foreign researchers have extensively investigated gas solubility, selective absorption mechanisms, and molecular transport in ionic liquids. Blanchard, Brennecke, Maginn, and co-workers studied the phase behavior of CO₂ in ionic liquids, free-energy profiles at gas-liquid interfaces, and absorption mechanisms. MacFarlane, Huang, Peng, Gupta, Jiang, Weber, and Kirchner analyzed the viscosity, structure, and CO₂ absorption properties of cyano-functionalized ionic liquids using experimental and computational methods.

Researchers in Uzbekistan have also investigated the properties and practical applications of ionic liquids as functional materials. In particular, E. Berdimurodov and co-workers analyzed the thermal stability and viscosity of ionic liquids and their use in nanocomposites as environmentally friendly lubricants. A.B. Ibragimov and co-workers demonstrated that MIL-101 composites modified with aminopolycarboxylate ionic liquids can significantly enhance CO₂ adsorption and CO₂/N₂ selectivity.

However, systematic molecular-level studies of the absorption and transport mechanisms of CO₂, H₂S, and CH₄ in cyano-functionalized imidazolium ionic liquids remain insufficient.

Connection of the topic of the dissertation with the scientific research activities of the organization where the dissertation was carried out. The dissertation research was conducted in accordance with the scientific research activities of the Institute of Materials Science of the Academy of Sciences of the Republic of Uzbekistan, within the framework of the fundamental project No. FZ-2020092817 entitled “Transport of Reactive Oxygen and Nitrogen Species through Plant Aquaporin Channels: An Atomic-Level Investigation”

The aim of the research is to determine the absorption and transport mechanisms of carbon dioxide, hydrogen sulfide, and methane in cyano-functionalized imidazolium-based ionic liquids using molecular dynamics methods.

The tasks of the research:

to construct models of [EMIM][SCN], [EMIM][DCA], [BMIM][SCN], and [BMIM][DCA] ionic liquids together with CO₂, H₂S, and CH₄ gas molecules, equilibrate the systems, and assess the reliability of the selected force-field parameters by comparing the calculated density values with experimental data;

to determine the free-energy profiles of CO₂, H₂S, and CH₄ in [EMIM][SCN], [EMIM][DCA], [BMIM][SCN], and [BMIM][DCA] ionic liquids using umbrella

sampling and WHAM, as well as the free-energy barriers for transfer from the interface to the bulk phase and their temperature dependence;

to determine the spatial distributions of gas molecules at the ionic-liquid interface and in the bulk phase using density profiles, and to characterize the local structural organization and relative spatial arrangement of selected gas-ion and ion-ion pairs using radial distribution functions;

to calculate the diffusion coefficients of CO₂, H₂S, and CH₄ molecules in the studied ionic liquids and determine their dependence on temperature, anion type, and cation alkyl-chain length;

to determine the effects of anion type and cation alkyl-chain length on gas absorption and transport properties through comparative analysis of free-energy, density-distribution, radial-distribution-function, and diffusion results.

The objects of the research are gas-ionic liquid systems consisting of [EMIM][SCN], [EMIM][DCA], [BMIM][SCN], and [BMIM][DCA] ionic liquids together with CO₂, H₂S, and CH₄ gas molecules.

The subject of the research comprises the thermodynamic stability, spatial distribution, local structural interactions, and molecular diffusion behavior of CO₂, H₂S, and CH₄ at the interface and in the bulk phase of [EMIM][SCN], [EMIM][DCA], [BMIM][SCN], and [BMIM][DCA] ionic liquids.

The methods of the research. Molecular dynamics simulations were used to investigate the thermodynamic, structural, and transport properties of CO₂, H₂S, and CH₄ in cyano-functionalized imidazolium-based ionic liquids. All calculations were performed using the GROMACS software package. Force-field parameters for the ionic liquids and gas molecules were adopted from molecular models reported in the literature, and the reliability of the selected models was assessed by comparing the calculated densities with available experimental data.

The gas-ionic liquid systems were constructed as slab models and subjected to energy minimization and equilibration. Free-energy profiles for the transfer of gas molecules from the vacuum region into the bulk phase of the ionic liquid were determined using umbrella sampling and WHAM. Density distributions, radial distribution functions, mean squared displacements, and diffusion coefficients were calculated from the simulation trajectories.

The scientific novelty of the research is in the following:

the free-energy profiles for the transfer of CO₂, H₂S, and CH₄ molecules from the vacuum region into the interface and the bulk phase of cyano-functionalized imidazolium-based [EMIM][SCN], [EMIM][DCA], [BMIM][SCN], and [BMIM][DCA] ionic liquids were determined.

the general thermodynamic trend of the gases in the studied ionic liquids was established in the order H₂S > CO₂ > CH₄; H₂S molecules were found to be more strongly stabilized in the bulk phase, whereas CO₂ molecules showed stronger stabilization at the gas-ionic liquid interface;

The dependence of the free-energy barriers for the transfer of CO₂, H₂S, and CH₄ molecules from the interface to the bulk phase on gas type, anion identity, and temperature was determined. H₂S transfer from the interface to the bulk phase in SCN⁻-based ionic liquids occurred with a lower free-energy barrier than in DCA⁻-based systems, whereas CH₄ transfer into the bulk phase was thermodynamically unfavorable in all investigated systems;

The anion-dependent spatial distribution patterns of gas molecules in ionic liquids were determined. CO₂ was found to accumulate preferentially at the interface in both anion-based systems; H₂S showed a relatively more uniform distribution throughout the bulk phase in SCN⁻-based systems, whereas it accumulated more strongly at the interface in DCA⁻-based systems; CH₄ was found to accumulate predominantly at the interface.

Extension of the cation alkyl chain from [EMIM]⁺ to [BMIM]⁺ did not alter the qualitative thermodynamic behavior of CO₂, H₂S, and CH₄, but resulted in lower molecular diffusion coefficients. Gas mobility was higher in DCA⁻-based ionic liquids than in the corresponding SCN⁻-based systems.

Practical results of the research are as follows:

a computational approach combining molecular dynamics simulations, umbrella sampling, density-profile analysis, radial distribution functions, and diffusion calculations was established for the molecular-level evaluation of the absorption and transport properties of CO₂, H₂S, and CH₄ in cyano-functionalized imidazolium ionic liquids;

a numerical dataset comprising the free-energy profiles, interfacial and bulk-phase distributions, and molecular diffusion coefficients of CO₂, H₂S, and CH₄ in [EMIM][SCN], [EMIM][DCA], [BMIM][SCN], and [BMIM][DCA] ionic liquids was established. These data can be used for comparative evaluation of gas absorption, selectivity, and transport properties in ionic liquids;

the results obtained on the effects of anion type and cation alkyl-chain length on the thermodynamic stability, local structural organization, and molecular mobility of the gases can be used for the preliminary molecular screening of promising ionic-liquid systems for the separation of CO₂ and H₂S from CH₄;

based on the research results, scientific and methodological recommendations were developed for the molecular-level evaluation of gas absorption and transport in cyano-functionalized imidazolium ionic liquids and for the selection of promising ionic liquids for natural-gas purification.

Reliability of the research results is ensured by the use of modern atomistic molecular dynamics simulations to investigate the absorption and transport properties of CO₂, H₂S, and CH₄ in imidazolium-based ionic liquids, umbrella sampling and the weighted histogram analysis method (WHAM) to determine free-energy profiles, as well as calculations performed using the GROMACS software package, which is widely used in international scientific practice. The reliability of the selected molecular models was evaluated by comparing the calculated densities

of the ionic liquids with available experimental data, and good agreement between the calculated and experimental values was established. The reliability of the obtained results is further supported by independent replicate simulations and by the internal consistency among the free-energy profiles, density distributions, radial distribution functions, and molecular diffusion results. The research findings were also presented and discussed at national and international scientific conferences and published in scientific journals recommended by the Higher Attestation Commission of the Republic of Uzbekistan, as well as in international journals indexed in the Scopus and Web of Science databases.

Scientific and practical significance of the research results lies in the possibility of using the obtained molecular dynamics results and the applied computational approach for the preliminary selection and evaluation of cyano-functionalized ionic liquids for natural-gas separation/purification. The results concerning the effects of anion type, cation alkyl-chain length, and temperature on gas thermodynamics and transport provide a scientific basis for selecting promising ionic-liquid systems for subsequent experimental investigation.

The practical significance of the research results lies in the possibility of using the obtained molecular dynamics results and the developed computational protocol for the preliminary selection and evaluation of cyano-functionalized ionic liquids for natural-gas purification. The results concerning the effects of anion type, cation chain length, and temperature on gas absorption and transport can serve as a scientific basis for designing new ionic-liquid absorbents, improving selectivity, and selecting regeneration conditions.

Implementation of the research results. The molecular dynamics results obtained within the dissertation on the absorption and transport of CO₂, H₂S, and CH₄ in imidazolium-based ionic liquids have been officially confirmed as being used in the research activities of the Research Centre for Carbon Dioxide Capture and Utilisation (CCDCU) at Sunway University, Malaysia (15 August 2025).

Furthermore, an article published in an international scientific journal indexed in the Scopus database on the basis of the research results has received 8 citations, demonstrating the scientific significance and recognition of the obtained results within the international scientific community.

Approbation of the research results. The results of this research were discussed at 2 international and 2 national scientific and practical conferences.

Publication of the research results. A total of 8 scientific works have been published on the dissertation topic. The main scientific results of the dissertation have been published in 4 scientific articles, including 2 articles in national scientific journals recommended by the Higher Attestation Commission of the Republic of Uzbekistan and 2 articles in international scientific journals indexed in the Scopus and Web of Science databases.

Structure and volume of the dissertation. The dissertation consists of an introduction, four chapters, a conclusion, a list of references, and appendices. The total volume of the dissertation is approximately 120 pages.

MAIN CONTENT OF THE DISSERTATION

The Introduction substantiates the relevance and necessity of the research, describes its aim, objectives, object, and subject, and demonstrates its compliance with national priorities for science and technology development. The scientific novelty and practical results are presented, the scientific and practical significance and reliability of the findings are explained, and information is provided on implementation, approbation, publications, and the structure of the dissertation.

The first chapter, entitled “Natural Gas Purification from Acidic Components Using Ionic Liquids and the Molecular Basis of Gas Absorption,” analyzes the physicochemical properties and industrial significance of the principal natural-gas components, carbon dioxide (CO_2), hydrogen sulfide (H_2S), and methane (CH_4), as well as their roles in gas-separation processes. The quadrupole moment of CO_2 , the dipole moment and high polarizability of H_2S , and the nonpolar character of CH_4 , which interacts mainly through weak van der Waals forces, are discussed as key molecular factors governing interactions with ionic liquids.

The chapter also reviews the main industrial technologies used to remove acidic components from natural gas, including aqueous amine absorption, physical solvents, membrane separation, and adsorption processes. The high regeneration energy, corrosion, solvent degradation, and volatility associated with amine absorbents; the dependence of physical solvents on high-pressure conditions; and the selectivity and stability limitations of membrane and adsorption technologies are examined. Based on this analysis, the need for alternative absorbents with low volatility, physical regenerability, and chemical stability is substantiated.

The role of imidazolium-based ionic liquids in gas-separation processes is also discussed, with emphasis on their low vapor pressure, thermal stability, structural tunability, and the effects of anion and cation composition on gas absorption. The ability of cyano-functionalized anions, particularly thiocyanate (SCN^-) and dicyanamide (DCA^-), to interact with CO_2 and H_2S , as well as their effects on viscosity and gas diffusion, is analyzed. The literature review demonstrates that comparative studies of CO_2 , H_2S , and CH_4 in $[\text{EMIM}][\text{SCN}]$, $[\text{EMIM}][\text{DCA}]$, $[\text{BMIM}][\text{SCN}]$, and $[\text{BMIM}][\text{DCA}]$ using a unified computational approach remain insufficient.

The second chapter, entitled “Computational Methods and Details of Molecular Modeling,” presents the theoretical foundations of molecular dynamics simulations, classical molecular mechanics, force fields, boundary conditions, thermodynamic ensembles, cutoff restrictions, and approaches for calculating long-range electrostatic interactions. The procedure for performing atomistic molecular dynamics simulations with the GROMACS software package, including system preparation, energy minimization, equilibration, and production runs, is described.

The chapter also describes the construction of gas-ionic liquid slab systems, the selection of force-field parameters for ionic liquids and gas molecules, the geometry of the simulation boxes, and the vacuum and gas-liquid interface models. Molecular models were prepared for $[\text{EMIM}][\text{SCN}]$, $[\text{EMIM}][\text{DCA}]$, $[\text{BMIM}][\text{SCN}]$, and $[\text{BMIM}][\text{DCA}]$, and computational systems were constructed to study the transfer

of CO₂, H₂S, and CH₄ through the ionic-liquid interface into the bulk phase (Figure 1).

The methodology for calculating potential-of-mean-force profiles using umbrella sampling is also presented. The reaction coordinate was defined as the movement of a gas molecule along the direction normal to the interface from the vacuum region toward the ionic-liquid bulk phase. Free-energy profiles for each gas were determined using WHAM. Procedures for calculating gas-density distributions, radial distribution functions, and molecular diffusion coefficients are also described.

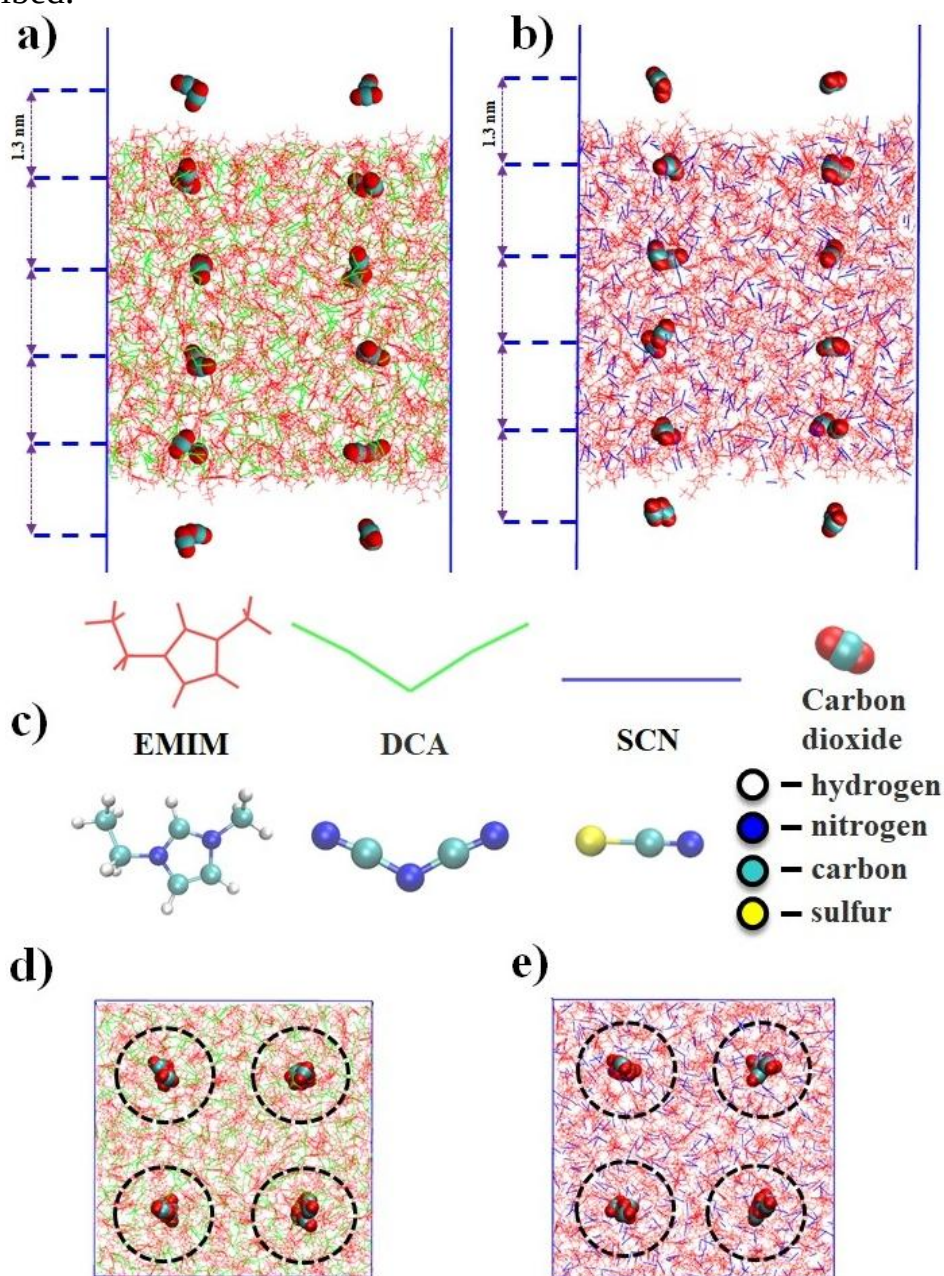


Figure 1. (a, b) Side and (d, e) top view of EMIMDCA (a, d) and EMIMSCN (b, e) ILs with embedded CO₂ molecules. These molecules are located at a 1.3 nm distance apart along the z-axis. Slabs of (c) optimized structures of [EMIM], [DCA] and [SCN] molecules. The CO₂ molecules were positioned at approximately 1.3 nm intervals along the z-axis.

The third chapter, entitled “Absorption Behavior of CO₂, H₂S, and CH₄ in [EMIM][SCN] and [EMIM][DCA] Ionic Liquids,” analyzes the thermodynamic, structural, and transport properties of the gases in two [EMIM]-based ionic liquids using molecular dynamics simulations. Free-energy profiles for CO₂, H₂S, and CH₄ in [EMIM][SCN] and [EMIM][DCA] were calculated at 298, 303, 353, and 373 K. The results show that interfacial adsorption and transfer into the bulk phase depend on both temperature and anion type.

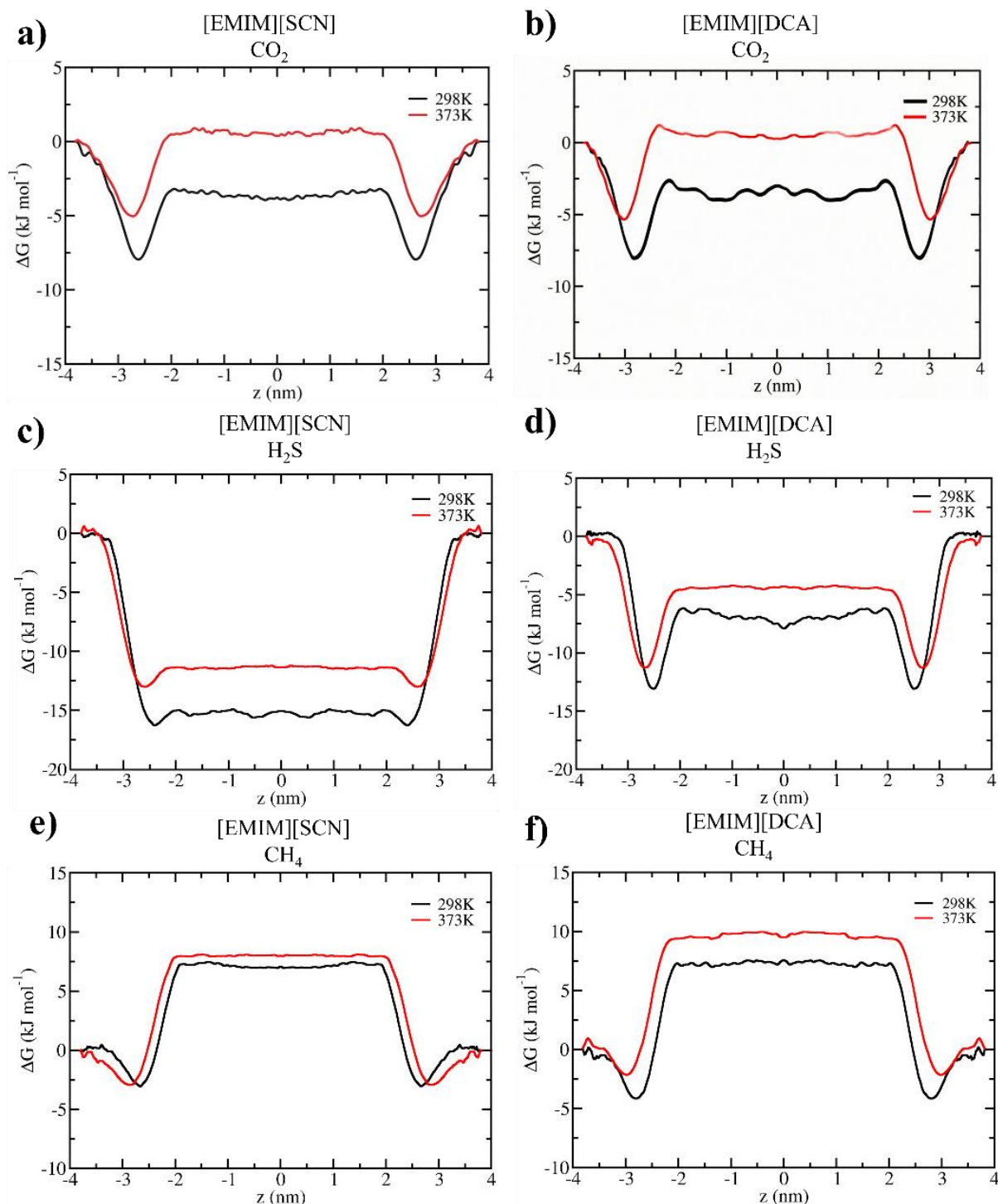


Figure 2. Free energy profiles (a,b) CO₂, (c,d) H₂S, and (e,f) CH₄ molecules in [EMIM][SCN] and [EMIM][DCA] ionic liquids at 298 K and 373 K.

Free-energy profiles for CO₂ showed negative interfacial minima in both ionic liquids. At 298 K, the interfacial free-energy minimum of CO₂ was approximately -7.6 kJ·mol⁻¹ in [EMIM][SCN] and -7.7 kJ·mol⁻¹ in [EMIM][DCA], while the corresponding bulk-phase free energies were -3.1 and -2.5 kJ·mol⁻¹, respectively. With increasing temperature, CO₂ stabilization in the bulk phase generally decreased. These results indicate thermodynamically favorable stabilization of CO₂ at both the interface and in the bulk phase of the two ionic liquids at 298 K.

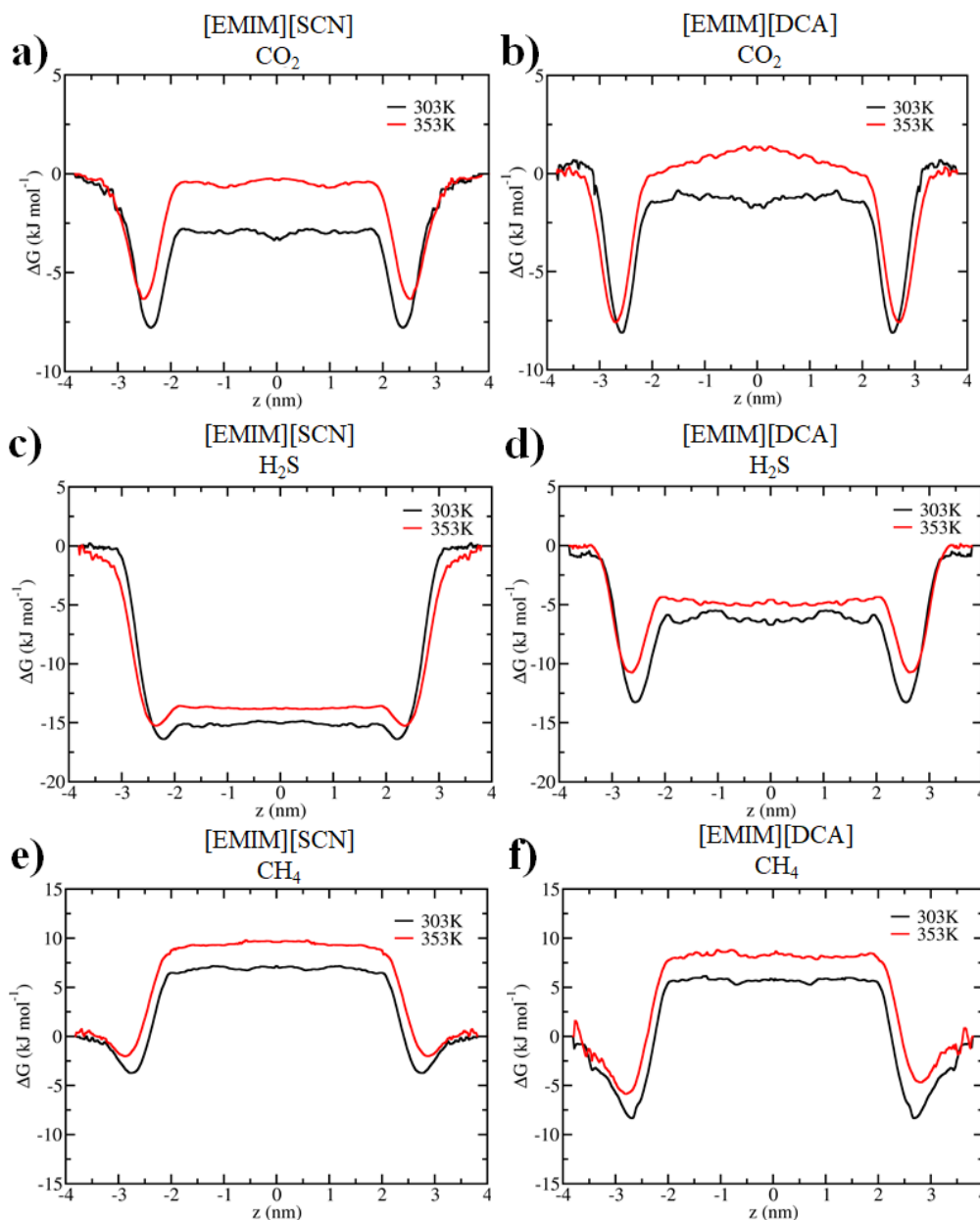


Figure 3. Free energy profiles of CO₂, H₂S, and CH₄ molecules in [EMIM][SCN] and [EMIM][DCA] ionic liquids at 303 K and 353 K.

H₂S exhibited the most favorable thermodynamic behavior among the investigated gases. At 298 K, the interfacial and bulk-phase free-energy values of H₂S in [EMIM][SCN] were -16.3 and -14.9 kJ·mol⁻¹, respectively. The interface-to-bulk free-energy barrier in this system was 1.4 kJ·mol⁻¹, indicating thermodynamically favorable transfer of H₂S into the bulk phase. Although H₂S was

strongly stabilized at the interface in [EMIM][DCA], its bulk-phase stabilization was weaker than that in [EMIM][SCN].

CH₄ exhibited weak negative interfacial minima in both ionic liquids, whereas its bulk-phase free-energy values were positive at all investigated temperatures. The interface-to-bulk free-energy barriers exceeded 10 kJ·mol⁻¹, with the highest value of 14.7 kJ·mol⁻¹ observed in [EMIM][DCA] at 303 K. These results indicate that the transfer of CH₄ into the ionic-liquid bulk phase is thermodynamically unfavorable.

The third chapter also analyzes the density distributions of gas molecules at the interface and in the bulk phase (see Figure 4). The density profiles showed that CO₂ accumulated mainly at the gas-ionic liquid interface, H₂S penetrated more deeply into the bulk phase, particularly in SCN⁻-based systems, whereas CH₄ was distributed mainly in the gas phase and near the interface.

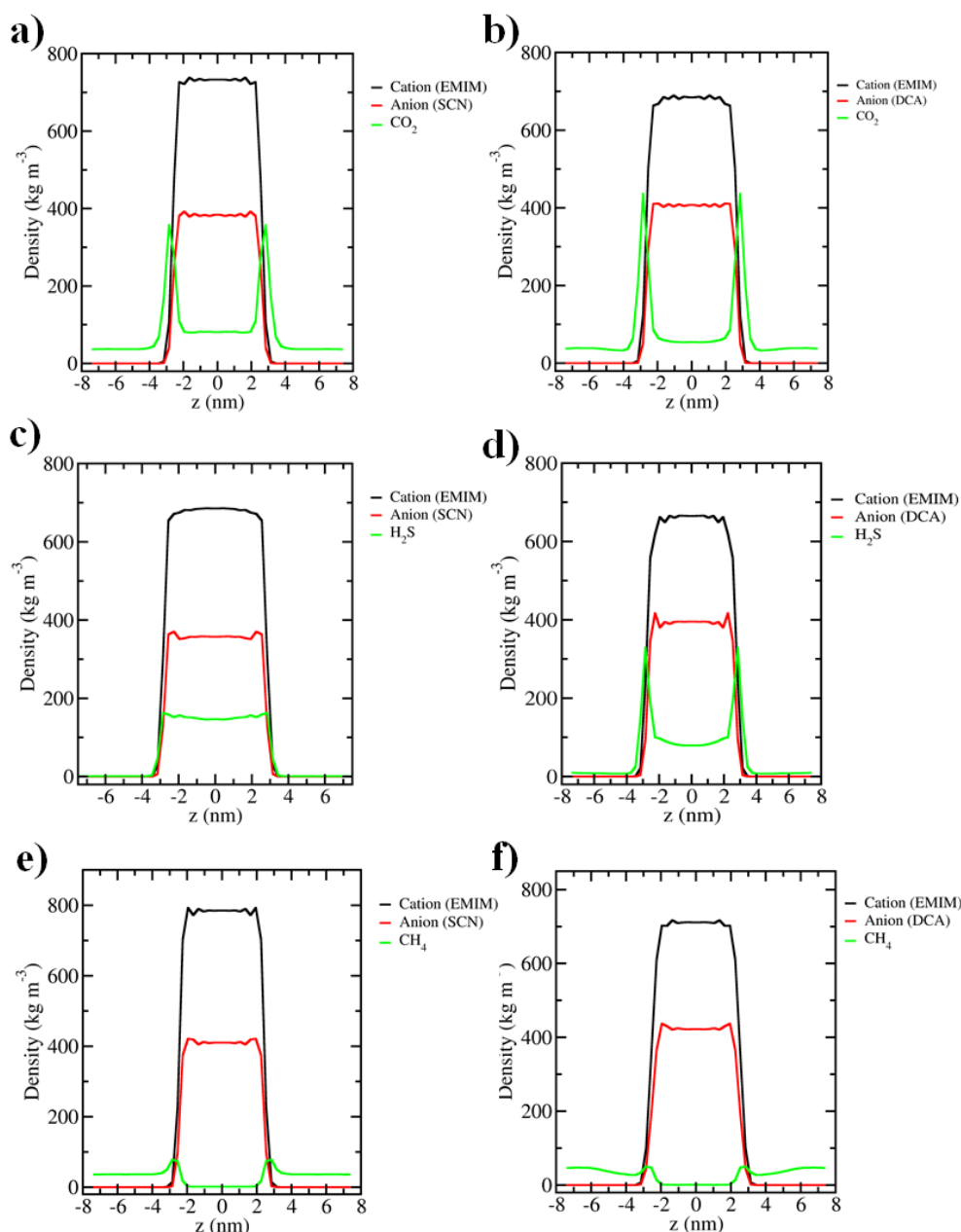


Figure 4. Density distribution profiles of CO₂, H₂S, and CH₄ molecules along the z-axis in ionic liquids.

Radial distribution function analysis was used to evaluate the local structural organization of cation-anion pairs in [EMIM][SCN] and [EMIM][DCA]. The introduction of CO₂, H₂S, or CH₄ caused no pronounced shift in the positions of the main cation-anion RDF peaks, indicating that gas loading did not substantially disrupt the short-range cation-anion organization of the ionic liquids.

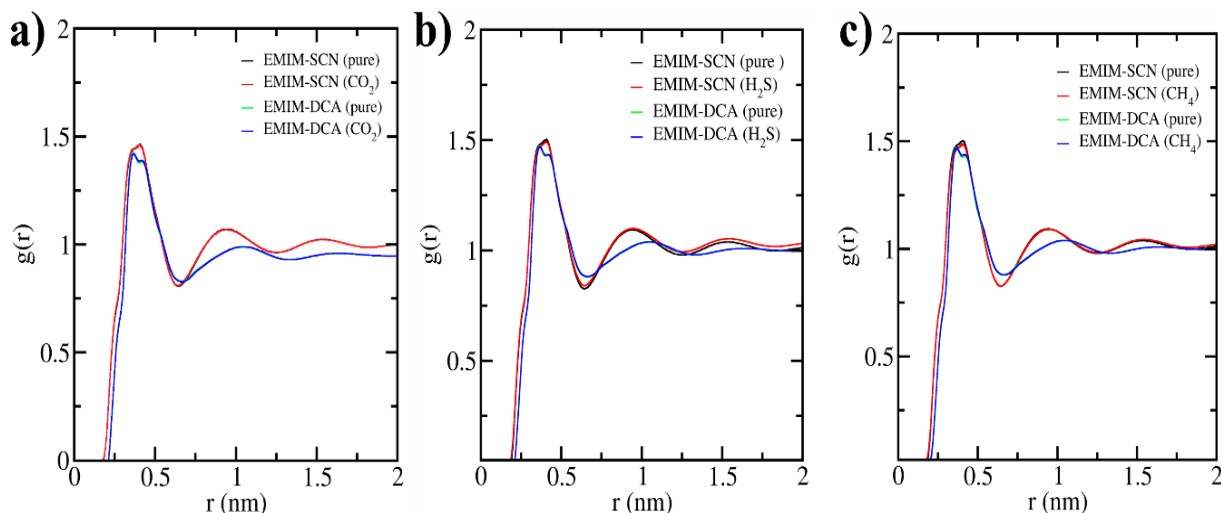


Figure 5. Radial distribution functions, $g(r)$, between EMIM⁺ cations and SCN⁻ or DCA⁻ anions in pure and gas-containing [EMIM][SCN] and [EMIM][DCA] systems at 298 K: (a) CO₂, (b) H₂S, and (c) CH₄.

The molecular diffusion coefficients of CO₂, H₂S, and CH₄ in [EMIM][SCN] and [EMIM][DCA] were also calculated (Table 1). The diffusion coefficients of all gases increased with increasing temperature. CH₄ generally exhibited the highest molecular mobility. The relative diffusion behavior of CO₂ and H₂S varied depending on anion type, gas-anion interactions, and temperature. The molecular mobility of the gases in DCA⁻-based ionic liquids was generally higher than that in the corresponding SCN⁻-based systems. The highest diffusion coefficient, $2.78 \times 10^{-5} \text{ cm}^2 \cdot \text{s}^{-1}$, was obtained for CH₄ in [EMIM][DCA] at 373 K.

Table 1.
Self-diffusion coefficients of CO₂, H₂S, and CH₄ molecules in [EMIM][SCN] and [EMIM][DCA] ionic liquids ($D \times 10^{-5} \text{ cm}^2 \cdot \text{s}^{-1}$).

Ionic liquid	CO ₂		H ₂ S		CH ₄	
	298K	373K	298K	373K	298K	373K
[EMIM][SCN]	0.2519 ± 0.003	0.9430 ± 0.001	0.2249 ± 0.004	1.1904 ± 0.002	0.4000 ± 0.002	1.2460 ± 0.001
[EMIM][DCA]	0.4743 ± 0.004	1.9327 ± 0.005	0.2768 ± 0.002	1.9625 ± 0.003	0.9700 ± 0.006	2.7800 ± 0.004

The fourth chapter, entitled “Absorption and Transport Behavior of CO₂, H₂S, and CH₄ in [BMIM][SCN] and [BMIM][DCA] Ionic Liquids,” analyzes the free-energy profiles, density distributions, radial distribution functions, and diffusion coefficients of the gases at 298 and 373 K. The obtained results were compared with the corresponding [EMIM]-based systems to evaluate the effect of cation alkyl-chain length.

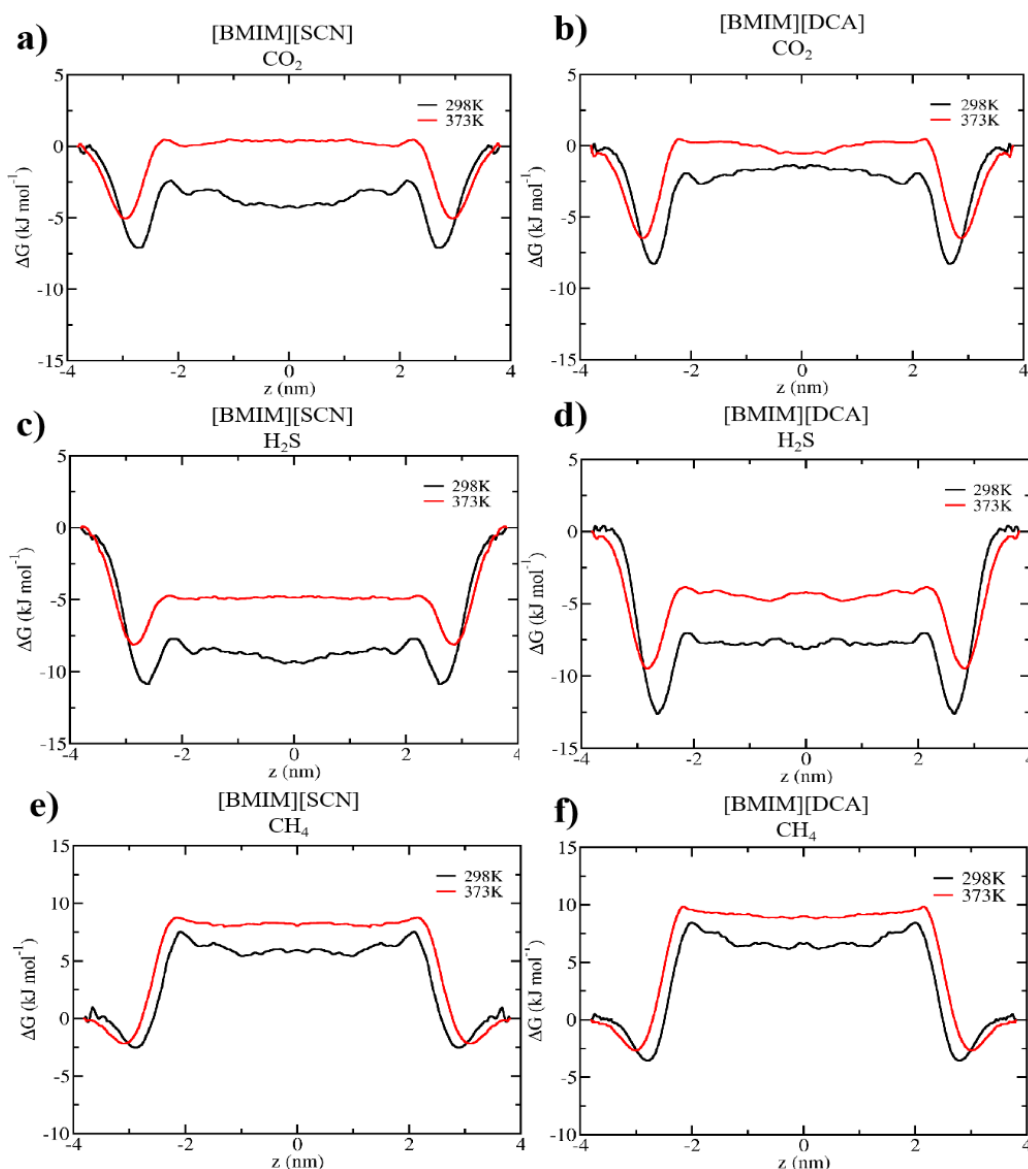


Figure 6. FEPs of CO₂, H₂S, and CH₄ molecules in [BMIM][SCN] and [BMIM][DCA] ionic liquids: (a) [BMIM][SCN] and (b) [BMIM][DCA] for CO₂; (c) [BMIM][SCN] and (d) [BMIM][DCA] for H₂S; (e) [BMIM][SCN] and (f) [BMIM][DCA] for CH₄.

At 298 K, the interfacial free-energy minima of CO₂ were -7.4 kJ·mol⁻¹ in [BMIM][SCN] and -8.0 kJ·mol⁻¹ in [BMIM][DCA]. The corresponding bulk-phase values were -2.45 and -1.5 kJ·mol⁻¹, respectively. The interface-to-bulk free-energy barriers were 4.9 and 6.5 kJ·mol⁻¹ in [BMIM][SCN] and [BMIM][DCA], respectively. At 373 K, the bulk-phase free-energy values approached zero, reaching 0.50 kJ·mol⁻¹ in both [BMIM][SCN] and [BMIM][DCA].

H₂S also exhibited more favorable thermodynamic behavior than CO₂ and CH₄ in the investigated [BMIM]-based systems. At 298 K, the interfacial free-energy values were -11.2 kJ·mol⁻¹ in [BMIM][SCN] and -12.7 kJ·mol⁻¹ in [BMIM][DCA]. The corresponding bulk-phase values were -7.6 and approximately -7.0 kJ·mol⁻¹, respectively. The interface-to-bulk free-energy barriers were 3.6 kJ·mol⁻¹ in [BMIM][SCN] and 5.7 kJ·mol⁻¹ in [BMIM][DCA].

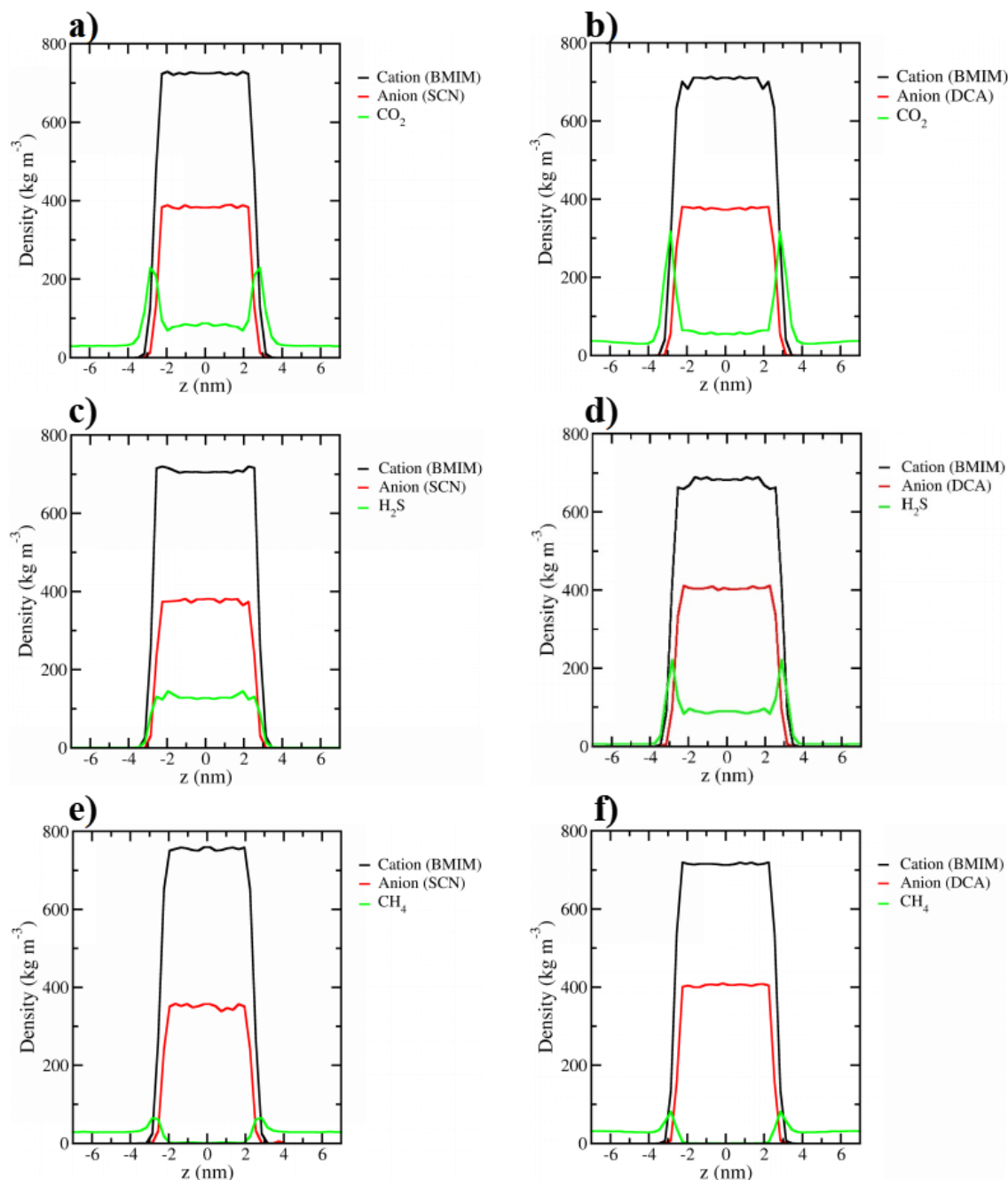


Figure 7. Density profiles of CO₂, H₂S, and CH₄ molecules in [BMIM][SCN] and [BMIM][DCA] ionic liquids

For CH₄, transfer into the bulk phase of both [BMIM][SCN] and [BMIM][DCA] was characterized by positive free-energy values. At 298 K, the interface-to-bulk free-energy barriers were 10.2 kJ·mol⁻¹ in [BMIM][SCN] and 11.3

$\text{kJ}\cdot\text{mol}^{-1}$ in [BMIM][DCA]. These results indicate that the transfer of CH_4 into the bulk phase is thermodynamically unfavorable.

The fourth chapter also analyzes density-distribution profiles, radial distribution functions, and diffusion coefficients. The density profiles showed the interfacial affinity of CO_2 and H_2S , deeper penetration of H_2S into the bulk phase in selected systems, and the distribution of CH_4 mainly in the gas phase and near the interface. Radial distribution functions showed that SCN^- and DCA^- anions formed different local structural correlations with the gas molecules.

The diffusion coefficients increased significantly for all gases with increasing temperature. At 298 K, the diffusion coefficient of CH_4 was $0.190 \times 10^{-5} \text{ cm}^2\cdot\text{s}^{-1}$ in [BMIM][SCN] and $0.438 \times 10^{-5} \text{ cm}^2\cdot\text{s}^{-1}$ in [BMIM][DCA]. At 373 K, these values increased to 1.261×10^{-5} and $1.770 \times 10^{-5} \text{ cm}^2\cdot\text{s}^{-1}$, respectively. Replacing $[\text{EMIM}]^+$ with $[\text{BMIM}]^+$ did not alter the general thermodynamic order of the gases but generally reduced their molecular mobility.

Table 2.

Self-diffusion coefficients of CO_2 , H_2S , and CH_4 molecules in [BMIM][SCN] and [BMIM][DCA] ionic liquids.

Ionic Liquid	$D \times 10^{-5} \text{ cm}^2\cdot\text{s}^{-1}$					
	CO_2		H_2S		CH_4	
	298 K	373 K	298 K	373 K	298 K	373 K
[BMIM][SCN]	0.137 ± 0.002	0.675 ± 0.002	0.147 ± 0.004	0.766 ± 0.007	0.190 ± 0.005	1.261 ± 0.004
[BMIM][DCA]	0.151 ± 0.001	0.827 ± 0.005	0.215 ± 0.001	0.795 ± 0.007	0.438 ± 0.003	1.770 ± 0.001

Overall, the results of the fourth chapter showed that replacing [EMIM] with [BMIM] did not fundamentally change the general absorption order. H_2S remained the most favorably absorbed gas, CO_2 showed intermediate absorption, and CH_4 remained unfavorable for entry into the bulk phase. The effect of cation alkyl-chain

length was mainly related to diffusion and gas distribution in the bulk phase, whereas the anion played the dominant role in determining gas selectivity.

CONCLUSIONS

1. The calculated density values for the molecular models of [EMIM][SCN], [EMIM][DCA], [BMIM][SCN], and [BMIM][DCA] ionic liquids showed good agreement with the available experimental data, demonstrating the suitability of the selected force-field parameters for modeling the gas-ionic liquid systems.

2. The free-energy profiles for the transfer of CO₂, H₂S, and CH₄ from the vacuum region into the bulk phase of the ionic liquids were determined, and H₂S was found to exhibit the most favorable absorption thermodynamics among the investigated gases. At 298 K, the interfacial and bulk-phase free-energy values of H₂S in [EMIM][SCN] were -16.3 and -14.9 kJ·mol⁻¹, respectively, while the interface-to-bulk energy barrier was 1.4 kJ·mol⁻¹.

3. CO₂ was found to be more strongly stabilized at the interface than in the bulk phase in all the investigated ionic liquids. At 298 K, the lowest interfacial free-energy minimum of -8.0 kJ·mol⁻¹ was obtained in [BMIM][DCA]. CO₂ interfacial stabilization was found to be stronger in DCA--based ionic liquids than in the corresponding SCN⁻-based systems.

4. The transfer of CH₄ into the bulk phase was found to be thermodynamically unfavorable in all the investigated ionic liquids. Its bulk-phase free-energy values remained positive at all studied temperatures, while the interface-to-bulk energy barriers exceeded 10 kJ·mol⁻¹. These results demonstrated the thermodynamic trends of the investigated ionic liquids for H₂S and CO₂ over CH₄.

5. Density distribution analysis supported the free-energy results, showing that CO₂ predominantly accumulates at the gas-ionic liquid interface, H₂S penetrates more deeply into the bulk phase, particularly in SCN--based systems, whereas CH₄ is mainly distributed near the interface and the adjacent vacuum region.

6. The molecular diffusion of CO₂, H₂S, and CH₄ was found to depend significantly on temperature and ionic-liquid structure. Increasing the temperature from 298 to 373 K increased the diffusion coefficients of all gases, while the values in DCA--based ionic liquids were generally higher than those in the corresponding SCN--based systems. The highest diffusion coefficient, 2.78×10^{-5} cm²·s⁻¹, was obtained for CH₄ in [EMIM][DCA] at 373 K.

7. Based on the combined thermodynamic, structural, and transport results, SCN⁻-based ionic liquids were found to provide relatively favorable conditions for the transfer of H₂S into the bulk phase, whereas DCA⁻ based systems favored interfacial stabilization of CO₂ and higher molecular mobility of the gases. These findings provide a scientific and methodological basis for the preliminary molecular

screening of ionic liquids intended for the separation of CO₂ and H₂S from CH₄ and for the evaluation of promising systems for natural-gas purification.

**“TIQXMMI” MTU HUZURIDAGI FUNDAMENTAL VA AMALIY
TADQIQOTLAR INSTITUTI HUZURIDAGI
ILMIY DARAJALAR BERUVCHI
DSc.03/06.11.2025.K/FM.10.09 RAQAMLI ILMIY KENGASH**

FUNDAMENTAL VA AMALIY TADQIQOTLAR INSTITUTI

QODIROV AKBAR ISMOIL OG‘LI

**IMIDAZOL HOSILALARI ASOSIDAGI ION SUYUQLIKLARDA CO₂, H₂S
VA CH₄ GAZLARINING YUTILISHINI MOLEKULYAR DINAMIKA
USULLARI YORDAMIDA TADQIQ QILISH**

02.00.04-Fizik kimyo

**FIZIKA-MATEMATIKA FANLARI BO‘YICHA FALSAFA DOKTORI (PhD)
DISSERTATSIYASI AVTOREFERATI**

Toshkent 2026

Fizika-matematika fanlari bo'yicha falsafa doktori (PhD) dissertatsiyasi mavzusi Oliy ta'lim, fan va innovatsiyalar vazirligi huzuridagi Oliy attestatsiya komissiyasida B2026.2.PhD/FM1550 raqam bilan ro'yxatga olingan.

Dissertatsiya ishi "TIQXMMI" MTU huzuridagi Fundamental va amaliy tadqiqotlar institutida bajarilgan.

Dissertatsiya avtoreferati uch tilda (o'zbek, ingliz va rus (rezyume)) Ilmiy Kengash veb-sahifasi www.ifar.uz va "ZiyoNet" axborot-ta'lim portaliga (www.ziynet.uz) joylashtirilgan.

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Dissertatsiya avtoreferati 2026-yil "___"-_____ kuni tarqatildi.

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KIRISH (falsafa doktori (PhD) dissertatsiyasi annotatsiyasi)

Dissertatsiya mavzusining dolzarbligi va zarurati. Hozirda dunyoda tabiiy gazni qayta ishlash, kislotali gazlarni ajratish va gaz tozalashning energiya tejamkor texnologiyalarini rivojlantirish muhim ilmiy-amaliy yo'nalishlardan biri hisoblanadi. Tabiiy gaz tarkibida uchraydigan karbonat angidrid (CO_2) va vodorod sulfid (H_2S) gazlari uning yonish issiqligini kamaytiradi, quvur va texnologik uskunalarda korroziya jarayonlarini kuchaytiradi hamda ekologik va texnik xavfsizlikka jiddiy ta'sir ko'rsatadi. Shu bilan birga, metan (CH_4) tabiiy gazning asosiy foydali komponenti bo'lib, gazni tozalash jarayonida uni imkon qadar saqlab qolish muhim iqtisodiy ahamiyatga ega. Shu sababli CO_2 va H_2S ni CH_4 dan selektiv ajratish uchun samarali, barqaror va qayta tiklanuvchi absorbentlarni ishlab chiqish dolzarb hisoblanadi.

Hozirgi vaqtda CO_2 va H_2S ni ajratishda amin eritmalari, erituvchilar, membranalar va adsorbentlar qo'llaniladi, biroq ushbu usullar regeneratsiya energiyasi, korroziya, erituvchi yo'qotilishi, selektivlik va barqarorlik bilan bog'liq cheklolarga ega. Shu sababli past uchuvchan, kimyoviy barqaror va oson qayta tiklanadigan ion suyuqliklar istiqbolli alternativ absorbent sifatida qaralmoqda. Ayniqsa, SCN^- va DCA^- anionlariga ega imidazoliy ion suyuqliklar CO_2 va H_2S bilan selektiv o'zaro ta'sirlashishi mumkin. Biroq $[\text{EMIM}][\text{SCN}]$, $[\text{EMIM}][\text{DCA}]$, $[\text{BMIM}][\text{SCN}]$ va $[\text{BMIM}][\text{DCA}]$ sistemalarida CO_2 , H_2S va CH_4 ning yutilishi hamda molekulyar transportini yagona hisoblash metodologiyasi asosida qiyosiy o'rganish yetarli darajada amalga oshirilmagan.

Dunyoda gazlarning ion suyuqliklardagi eruvchanligi, diffuziyasi va molekulyar o'zaro ta'sirlarini o'rganish bo'yicha tajribaviy hamda hisoblash tadqiqotlariga katta e'tibor qaratilmoqda. Xususan, molekulyar dinamika simulyatsiyalari, soyabonli namunalash usuli, erkin energiya profillari, radial taqsimot funksiyasi va diffuziya koeffitsiyentlari yordamida gaz molekulalarining ion suyuqlik interfeysi va hajmiy fazadagi xatti-harakatini atom darajada baholash imkoniyati mavjud. Bunday yondashuvlar tajriba orqali bevosita kuzatish qiyin bo'lgan molekulyar mexanizmlarni aniqlashga, gaz-anion va gaz-kation o'zaro ta'sirlarining rolini baholashga hamda absorbentlarning selektivlik xususiyatlarini tushuntirishga xizmat qiladi.

Respublikamizda so'nggi yillarda molekulyar modellashtirish, fizik-kimyoviy jarayonlarni molekulyar darajada tahlil qilish, gazlar va suyuqliklar interfeysidagi transport hodisalarini o'rganish bo'yicha muhim ilmiy tadqiqotlar olib borilmoqda. Xususan, molekulyar dinamika, erkin energiya hisoblashlari, diffuziya va strukturaviy tahlil usullarining rivojlanishi tabiiy gazni tozalash, ekologik xavfsizlik, energiya samaradorligi va yangi funksional materiallarni ishlab chiqish yo'nalishlarida fundamental ilmiy asos yaratadi. Shu nuqtai nazardan, imidazoliy asosidagi sianid-funksional ion suyuqliklarda CO_2 , H_2S va CH_4 gazlarining yutilishini molekulyar dinamika usullari yordamida tadqiq qilish tabiiy gazni tozalash uchun yangi absorbentlarni baholashda muhim ilmiy-amaliy ahamiyatga ega.

O'zbekiston Respublikasi Prezidentining 2022-yil 28-yanvardagi "2022-2026-yillarga mo'ljallangan Yangi O'zbekistonning taraqqiyot strategiyasi to'g'risida"gi PF-60-sonli Farmoni, O'zbekiston Respublikasi Prezidentining 2020-yil 12-avgustdagi PQ-4805-sonli "Kimyo va biologiya yo'nalishlarida uzluksiz ta'lim sifatini va ilm-fan natijadorligini oshirish chora-tadbirlari to'g'risida"gi Qarori hamda mazkur faoliyatga tegishli boshqa me'yoriy-huquqiy hujjatlarda belgilangan vazifalarni amalga oshirishda ushbu dissertatsiya tadqiqoti muayyan darajada xizmat qiladi.

Tadqiqotning respublika fan va texnologiyalari rivojlanishining asosiy ustuvor yo'nalishlariga bog'liqligi. Mazkur tadqiqot respublika fan va texnologiyalar rivojlanishining VII "Kimyo texnologiyalari va nanotexnologiyalar" ustuvor yo'nalishiga muvofiq bajarilgan.

Muammoning o'rganilganlik darajasi. Xorijiy olimlar tomonidan ion suyuqliklarda gazlarning eruvchanligi, selektiv absorbsiya mexanizmlari va molekulyar transport jarayonlari keng o'rganilgan. Blanchard, Brennecke, Maginn va hamkorlari CO₂ ning ion suyuqliklardagi fazaviy xatti-harakati, gaz-suyuqlik interfeysidagi erkin energiya profillari va absorbsiya mexanizmlarini tadqiq qilgan. MacFarlane, Huang, Peng, Gupta, Jiang, Weber va Kirchner sianid-funksional ion suyuqliklarning qovushqoqligi, tuzilishi va CO₂ yutish xususiyatlarini tajribaviy hamda hisoblash usullari bilan tahlil qilgan.

Respublikamiz olimlari ishtirokida ion suyuqliklarning funksional materiallar sifatidagi xossalari va amaliy qo'llanilishiga oid tadqiqotlar olib borilmoqda. Xususan, E. Berdimurodov va hamkorlari ion suyuqliklarning termik barqarorligi, qovushqoqligi va nanokompozitlar tarkibida ekologik moylash materiallari sifatida qo'llanilishini tahlil qilgan. A.B. Ibragimov va hamkorlari esa aminopolikarboksilat ion suyuqliklari bilan modifikatsiyalangan MIL-101 kompozitlarining CO₂ adsorbsiyasi va CO₂/N₂ selektivligini sezilarli oshirish mumkinligini ko'rsatgan.

Biroq sianid-funksional imidazoliy ion suyuqliklarda CO₂, H₂S va CH₄ ning yutilishi hamda transport mexanizmlari molekulyar darajada yetarlicha o'rganilmagan.

Dissertatsiya mavzusining dissertatsiya bajarilgan ilmiy-tadqiqot muassasasining ilmiy-tadqiqot ishlari bilan bog'liqligi. Dissertatsiya tadqiqoti O'zbekiston Respublikasi Fanlar Akademiyasi Materialshunoslik instituti ilmiy tadqiqot ishlariga muvofiq FZ-2020092817 sonli "Reaktiv kislorod va azot zarralarining o'simlik akvaporin kanallari orqali kirishi: atomar darajadagi tadqiqot" nomli fundamental loyihasi doirasida amalga oshirilgan.

Tadqiqotning maqsadi — sianid-funksional imidazoliy asosidagi ion suyuqliklarda karbonat angidrid, vodorod sulfidi va metan gazlarining yutilish va transport mexanizmlarini molekulyar dinamika usullari yordamida aniqlash.

Tadqiqotning vazifalari:

[EMIM][SCN], [EMIM][DCA], [BMIM][SCN] va [BMIM][DCA] ion suyuqliklari hamda CO₂, H₂S va CH₄ gaz molekulalarining modellarini yaratish, tizimlarni muvozanat holatiga keltirish va tanlangan kuch maydoni parametrlarining ishonchliligini tajriba zichlik qiymatlari bilan taqqoslash orqali baholash;

soyabonli namunalash va VGQAU usuli yordamida CO_2 , H_2S va CH_4 molekulalarining [EMIM][SCN], [EMIM][DCA], [BMIM][SCN] va [BMIM][DCA] ion suyuqliklaridagi erkin energiya profillarini, interfeysdan hajmiy fazaga o'tish erkin energiya to'siqlarini hamda ushbu ko'rsatkichlarning haroratga bog'liqligini aniqlash;

gaz molekulalarining ion suyuqlik interfeysi va hajmiy fazadagi fazoviy taqsimotini zichlik profillari asosida aniqlash hamda radial taqsimot funksiyalari yordamida tanlangan gaz-ion va ion-ion juftliklarining lokal strukturaviy tuzilishi va o'zaro joylashuvini tavsiflash;

CO_2 , H_2S va CH_4 molekulalarining o'rganilgan ion suyuqliklardagi diffuziya koeffitsiyentlarini hisoblash hamda ularning harorat, anion turi va kation alkil zanjiri uzunligiga bog'liqligini aniqlash;

erkin energiya, zichlik taqsimoti, radial taqsimot funksiyasi va diffuziya natijalarini qiyosiy tahlil qilish asosida anion turi va kation alkil zanjiri uzunligining gazlarning yutilishi va transport xususiyatlariga ta'sirini aniqlash.

Tadqiqotning obyekti sifatida [EMIM][SCN], [EMIM][DCA], [BMIM][SCN] va [BMIM][DCA] ion suyuqliklari hamda CO_2 , H_2S va CH_4 gaz molekulalaridan tashkil topgan gaz-ion suyuqlik tizimlari tanlangan.

Tadqiqotning predmeti [EMIM][SCN], [EMIM][DCA], [BMIM][SCN] va [BMIM][DCA] ion suyuqliklarida CO_2 , H_2S va CH_4 gazlarining interfeys va hajmiy fazadagi termodinamik barqarorligi, fazoviy taqsimoti, lokal strukturaviy o'zaro ta'sirlari hamda molekulyar diffuziya xususiyatlaridan iborat.

Tadqiqotning usullari. Dissertatsiya ishida CO_2 , H_2S va CH_4 gazlarining sianid-funksional imidazoliy asosidagi ion suyuqliklardagi termodinamik, strukturaviy va transport xususiyatlarini o'rganish uchun molekulyar dinamika simulyatsiyalaridan foydalanilgan. Hisoblashlar GROMACS dasturiy paketi yordamida bajarilgan. Ion suyuqliklari va gaz molekulalari uchun kuch maydoni parametrlari ilmiy adabiyotlarda keltirilgan molekulyar modellardan olingan, tanlangan modellarning ishonchliligi esa hisoblangan zichliklarni tajriba ma'lumotlari bilan taqqoslash orqali baholangan.

Gaz-ion suyuqlik tizimlari qatlamli model ko'rinishida yaratilgan hamda energiya minimallashtirish va muvozanatlash bosqichlaridan o'tkazilgan. Gaz molekulalarining vakuumdan ion suyuqlikning hajmiy fazasiga o'tishidagi erkin energiya profillari soyabonli namunalash va vaznlangan gistogramma qiymatlari analizi uslubi (VGQAU) yordamida aniqlangan. Simulyatsiya trayektoriyalari asosida zichlik taqsimotlari, radial taqsimot funksiyalari, o'rtacha kvadratik siljishlar va diffuziya koeffitsiyentlari hisoblangan.

Tadqiqotning ilmiy yangiligi quyidagilardan iborat:

Sianid-funksional imidazoliy asosidagi [EMIM][SCN], [EMIM][DCA], [BMIM][SCN] va [BMIM][DCA] ion suyuqliklarida CO_2 , H_2S va CH_4 molekulalarining vakuum sohasidan interfeys va ion suyuqlik hajmiy fazasiga o'tish erkin energiya profillari hisoblangan;

o'rganilgan ion suyuqliklarda gazlarning termodinamik afzallik tartibi $H_2S > CO_2 > CH_4$ ekanligi, H_2S molekulalarining hajmiy fazada, CO_2 molekulalarining esa gaz-ion suyuqlik interfeysida nisbatan kuchliroq barqarorligi aniqlandi;

CO_2 , H_2S va CH_4 molekulalarining interfeysdan hajmiy fazaga o'tish erkin energiya to'siqlarining gaz turi, anion tabiati va haroratga bog'liqligi aniqlanib, SCN^- asosidagi ion suyuqliklarda H_2S ning interfeysdan hajmiy fazaga o'tishi DCA^- asosidagi tizimlarga nisbatan kichikroq erkin energiya to'sig'i bilan kechishi, CH_4 ning esa barcha o'rganilgan tizimlarda hajmiy fazaga o'tishi termodinamik jihatdan noqulay ekanligi ko'rsatilgan;

Gaz molekulalarining ion suyuqliklarda anion tabiatiga bog'liq fazoviy taqsimlanish qonuniyatlari aniqlanib, CO_2 ning ikkala anionli tizimda interfeysda ko'proq to'planishi, H_2S ning SCN^- asosidagi tizimlarda hajmiy faza bo'ylab nisbatan bir tekisroq taqsimlanishi, DCA^- asosidagi tizimlarda esa interfeysda ko'proq to'planishi, CH_4 ning asosan interfeysda to'planishi aniqlangan.

$[EMIM]^+$ kationidan $[BMIM]^+$ kationiga alkil zanjirining uzaytirilishi CO_2 , H_2S va CH_4 gazlarining sifat jihatdan umumiy termodinamik tendensiyasini o'zgartirmadi, biroq ularning molekulyar diffuziya koeffitsiyentlarining kamayishiga olib keldi. Gazlarning molekulyar harakatchanligi mos keluvchi SCN^- asosidagi ion suyuqliklarga nisbatan DCA^- asosidagi ion suyuqliklarda yuqoriroq bo'ldi.

Tadqiqotning amaliy natijalari quyidagilardan iborat:

CO_2 , H_2S va CH_4 gazlarining sianid-funksional imidazoliy ion suyuqliklarda yutilishi va transport xususiyatlarini molekulyar darajada baholashga imkon beruvchi molekulyar dinamika, soyabonli namunalash, zichlik profillari, radial taqsimot funksiyalari va diffuziya hisoblashlariga asoslangan hisoblash yondashuvi shakllantirilgan;

$[EMIM][SCN]$, $[EMIM][DCA]$, $[BMIM][SCN]$ va $[BMIM][DCA]$ ion suyuqliklarida CO_2 , H_2S va CH_4 gazlarining erkin energiya profillari, interfeys va hajmiy fazadagi taqsimoti hamda molekulyar diffuziya koeffitsiyentlarini qamrab oluvchi sonli ma'lumotlar majmuasi shakllantirilgan. Ushbu ma'lumotlardan gazlarning ion suyuqliklardagi yutilishi, selektivligi va transport xususiyatlarini qiyosiy baholashda foydalanish mumkin;

anion turi va kation alkil zanjiri uzunligining gazlarning termodinamik barqarorligi, lokal strukturaviy tashkil topishi va molekulyar harakatchanligiga ta'siri bo'yicha olingan natijalar CO_2 va H_2S ni CH_4 dan ajratish uchun istiqbolli ion suyuqlik tizimlarini dastlabki molekulyar saralashda qo'llanishi mumkin;

tadqiqot natijalari asosida sianid-funksional imidazoliy ion suyuqliklarda gazlarning yutilishi va transportini molekulyar darajada baholash hamda tabiiy gazni tozalash uchun istiqbolli ion suyuqliklarni tanlash bo'yicha ilmiy-uslubiy tavsiyalar ishlab chiqilgan.

Tadqiqot natijalarining ishonchliligi. CO_2 , H_2S va CH_4 gazlarining imidazoliy asosidagi ion suyuqliklarda yutilishi va transport xususiyatlarini o'rganishda zamonaviy molekulyar dinamika simulyatsiyalari, erkin energiya profillarini aniqlash uchun soyabonli namunalash va VGQAU usuli, shuningdek xalqaro ilmiy amaliyotda keng qo'llaniladigan GROMACS dasturiy paketi asosida

hisoblashlar bajarilgani bilan ta'minlangan. Tanlangan molekulyar modellarning ishonchliligi hisoblangan ion suyuqlik zichliklarini mavjud eksperimental ma'lumotlar bilan taqqoslash orqali baholanib, ularning yaxshi mos kelishi aniqlangan. Hisoblashlarning mustaqil takroriy simulyatsiyalar asosida bajarilgani hamda erkin energiya profillari, zichlik taqsimotlari, radial taqsimlanish funksiyalari va molekulyar diffuziya natijalarining o'zaro muvofiqligi olingan natijalarning ishonchliligini tasdiqlaydi. Tadqiqot natijalari respublika va xalqaro ilmiy-amaliy konferensiyalarda muhokamadan o'tkazilgani hamda O'zbekiston Respublikasi Oliy attestatsiya komissiyasi tomonidan tavsiya etilgan va xalqaro Scopus/Web of Science bazalarida indekslanuvchi ilmiy jurnallarda nashr etilgani bilan ham asoslanadi.

Tadqiqot natijalarining ilmiy va amaliy ahamiyati olingan molekulyar dinamika natijalari va qo'llanilgan hisoblash yondashuvidan tabiiy gazni ajratish/tozalash uchun sianid-funksional ion suyuqliklarni dastlabki tanlash va baholashda foydalanish imkoniyati bilan izohlanadi. Anion turi, kation alkil zanjiri uzunligi va haroratning gazlarning termodinamik hamda transport xususiyatlariga ta'siri bo'yicha olingan natijalar keyingi tajribaviy tadqiqotlar uchun istiqbolli ion suyuqlik tizimlarini tanlashga ilmiy asos bo'lib xizmat qiladi.

Tadqiqot natijalarining amaliy ahamiyati olingan molekulyar dinamika natijalari va shakllantirilgan hisoblash protokoli tabiiy gazni tozalash uchun sianid-funksional ion suyuqliklarni dastlabki tanlash va baholashda qo'llanishi mumkinligi bilan izohlanadi. Shuningdek, anion turi, kation zanjiri uzunligi va haroratning gaz yutilishi hamda transport xususiyatlariga ta'siri bo'yicha olingan natijalar yangi ion suyuqlik absorbentlarini loyihalash, selektivlikni oshirish va regeneratsiya sharoitlarini tanlashda ilmiy asos bo'lib xizmat qiladi.

Tadqiqot natijalarining joriy qilinishi:

Dissertatsiya doirasida CO_2 , H_2S va CH_4 gazlarining imidazoliy asosidagi ion suyuqliklarda yutilishi va transportiga oid olingan molekulyar dinamika natijalari Malayziyadagi Sunway universiteti huzuridagi "karbonat angidridni tutib qolish va undan foydalanish ilmiy-tadqiqot markazining" (CCDCU) ilmiy-tadqiqot faoliyatida qo'llanilgani rasman tasdiqlangan (2025-yil 15-avgust).

Tadqiqot natijalari asosida Scopus bazasida indekslanuvchi xalqaro ilmiy jurnalda chop etilgan maqolaga 8 ta iqtibos keltirilgani natijalarning xalqaro ilmiy hamjamiyatdagi ahamiyati va e'tirofini tasdiqlaydi.

Tadqiqot natijalarining aprobatsiyasi. Mazkur tadqiqot natijalari 2 ta xalqaro va 2 ta respublika ilmiy-amaliy anjumanlarida muhokamadan o'tkazilgan.

Tadqiqot natijalarining e'lon qilinganligi. Dissertatsiya mavzusi bo'yicha jami 8 ta ilmiy ish chop etilgan. Dissertatsiyaning asosiy ilmiy natijalari 4 ta ilmiy maqolada e'lon qilingan bo'lib, shulardan 2 tasi O'zbekiston Respublikasi Oliy attestatsiya komissiyasi tomonidan tavsiya etilgan respublika ilmiy jurnallarida va 2 tasi Scopus hamda Web of Science ma'lumotlar bazalarida indekslanuvchi xalqaro ilmiy jurnallarda chop etilgan.

Dissertatsiyaning tuzilishi va hajmi. Dissertatsiya tarkibi kirish qismi, to'rtta bob, xulosa, foydalanilgan adabiyotlar ro'yxati hamda ilovalardan iborat. Dissertatsiyaning umumiy hajmi 120 betni tashkil etadi.

DISSERTATSIYANING ASOSIY MAZMUNI

Kirish qismida o'tkazilgan tadqiqotlarning dolzarbligi va zarurati asoslangan, tadqiqotning maqsadi va vazifalari, obyekti va predmeti tavsiflangan, respublika fan va texnologiyalari rivojlanishining ustuvor yo'nalishlariga mosligi ko'rsatilgan. Tadqiqotning ilmiy yangiligi va amaliy natijalari bayon qilingan, olingan natijalarning ilmiy va amaliy ahamiyati ochib berilgan, tadqiqot natijalarining ishonchliligi, aprobatyasi, e'lon qilingan ishlar hamda dissertatsiya tuzilishi bo'yicha ma'lumotlar keltirilgan.

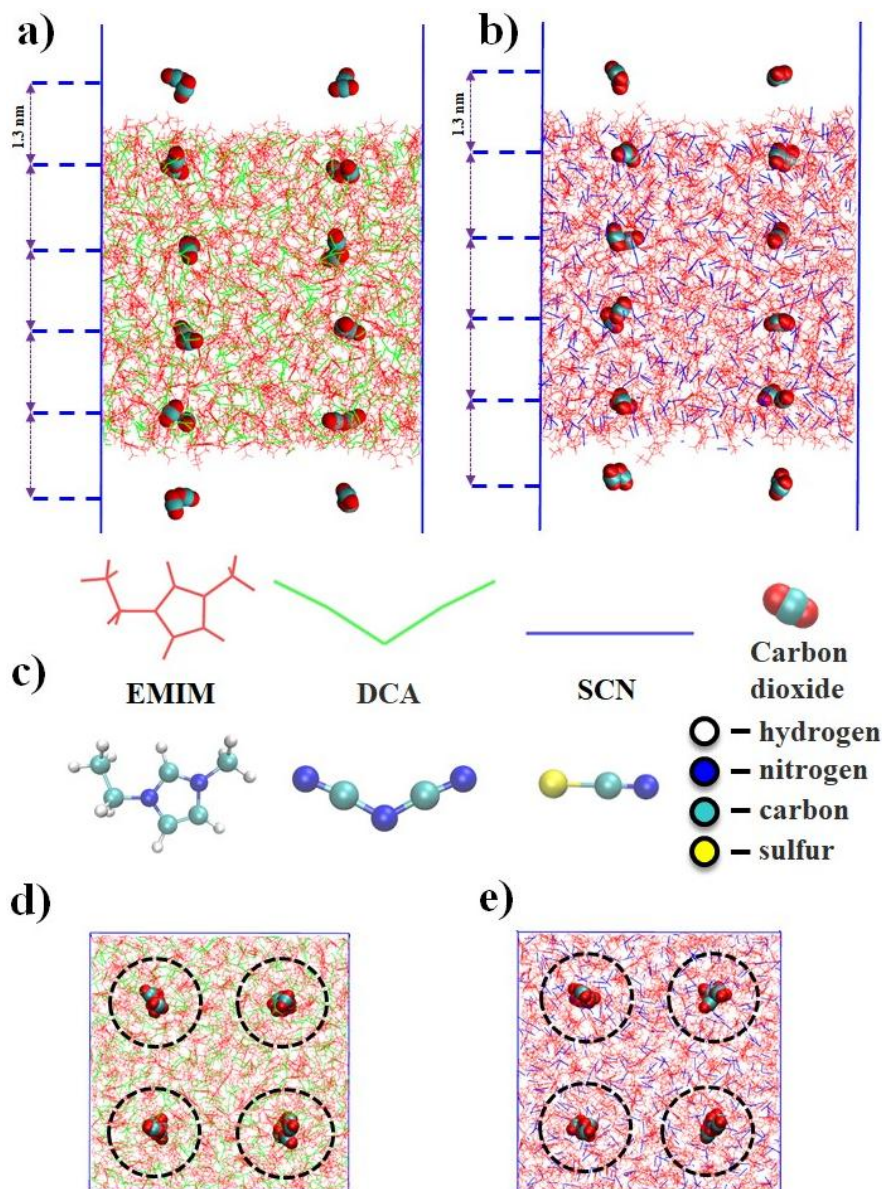
Dissertatsiyaning "Ion suyuqliklar yordamida tabiiy gazni nordon komponentlardan tozalash va gaz yutilishining molekulyar asoslari" deb nomlangan birinchi bobida tabiiy gaz tarkibidagi asosiy komponentlar — karbonat angidrid (CO_2), vodorod sulfid (H_2S) va metan (CH_4) ning fizik-kimyoviy xossalari, sanoatdagi ahamiyati hamda gaz ajratish jarayonlaridagi roli tahlil qilingan. CO_2 molekulasi kvadrupol momentga ega bo'lishi, H_2S ning dipol momenti va yuqori qutblanuvchanligi, CH_4 ning esa qutbsizligi hamda asosan zaif van-der-Vaals kuchlari orqali ta'sirlashishi gazlarning ion suyuqliklar bilan o'zaro ta'sirini belgilovchi muhim molekulyar omillar sifatida tahlil qilingan.

Mazkur bobda tabiiy gazni nordon komponentlardan tozalashda qo'llaniladigan asosiy sanoat texnologiyalari — suvli aminli absorbsiya tizimlari, fizik erituvchilar, membranali ajratish va adsorbsion jarayonlarning afzalliklari hamda cheklovlari tahlil qilingan. Aminli absorbentlarning yuqori regeneratsiya energiyasi, korroziya, erituvchi degradatsiyasi va uchuvchanlik bilan bog'liq kamchiliklari, fizik erituvchilarning yuqori bosim sharoitiga bog'liqligi, membranali va adsorbsion texnologiyalarning esa selektivlik hamda barqarorlik bo'yicha cheklovlari ko'rsatib berilgan. Ushbu tahlil asosida past uchuvchanlikka ega, fizik jihatdan qayta tiklanadigan va kimyoviy barqaror alternativ absorbentlarga ehtiyoj mavjudligi asoslangan.

Birinchi bobda, shuningdek, imidazoliy asosidagi ion suyuqliklarning gaz ajratish jarayonlaridagi o'rni, ularning past bug' bosimi, termik barqarorligi, strukturaviy sozlanishi va anion-kation tarkibining gaz yutilishiga ta'siri yoritilgan. Sianid-funksional anionlar, xususan tiotsianat (SCN^-) va disianamid (DCA^-) anionlarining CO_2 va H_2S bilan o'zaro ta'sirlashish imkoniyati, ularning qovushqoqlik, gaz diffuziyasiga ta'siri tahlil qilingan. Adabiyotlar tahlili asosida [EMIM][SCN], [EMIM][DCA], [BMIM][SCN] va [BMIM][DCA] ion suyuqliklarida CO_2 , H_2S va CH_4 gazlarining yutilishi bir xil hisoblash yondashuvi asosida qiyosiy o'rganilishi yetarli emasligi ko'rsatilgan.

Dissertatsiyaning "Hisoblash metodlari va molekulyar modellash tirish tafsilotlari" deb nomlangan ikkinchi bobida molekulyar dinamika simulyatsiyalarining nazariy asoslari, klassik molekulyar mexanika, kuch maydonlari, chegaraviy shartlar, termodinamik ansambllar, cutoff cheklovlari va

uzoq masofali elektrostatik o‘zaro ta’sirlarni hisoblash yondashuvlari bayon qilingan. GROMACS dasturiy paketi yordamida molekulyar dinamika simulyatsiyalarini bajarish tartibi, tizimlarni tayyorlash, energiyani minimallashtirish, muvozanatlashtirish va ishlab chiqarish bosqichlari haqida ma’lumot berilgan.



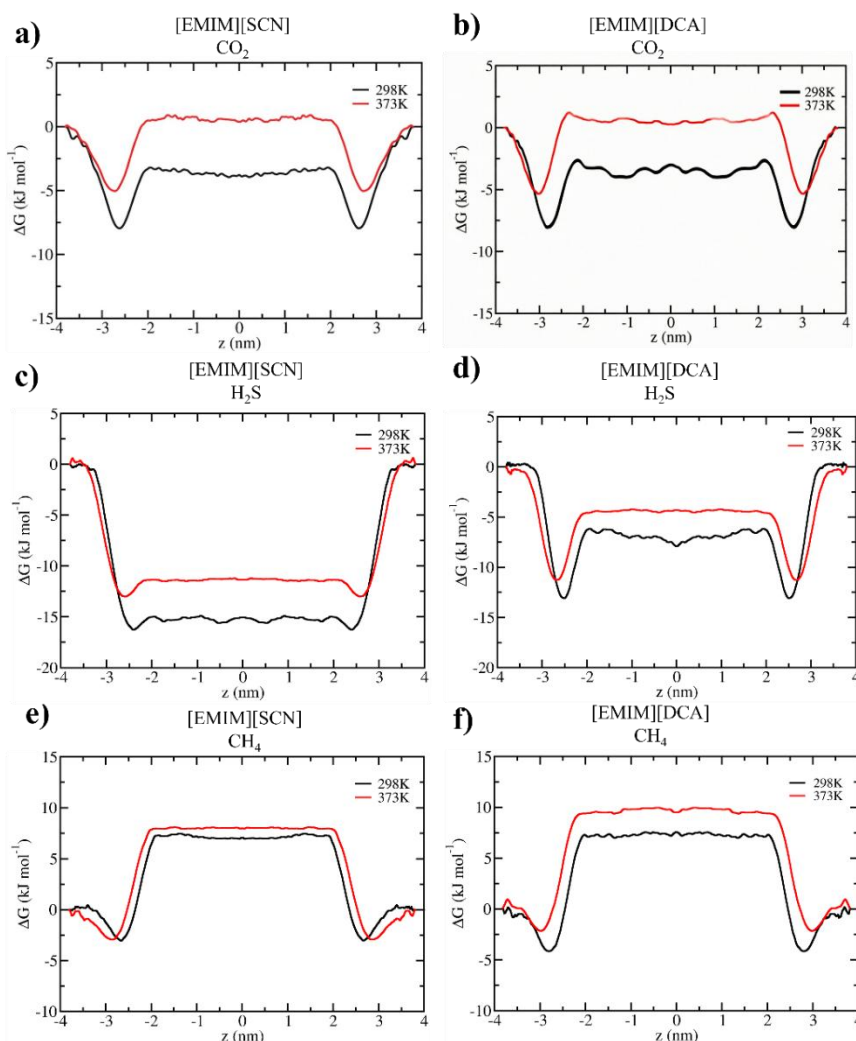
1-rasm. (a, b) CO₂ molekulalari joylashtirilgan EMIMDCA (a, d) va EMIMSCN (b, e) ion suyuqliklarining yon tomondan, (d, e) esa yuqoridan ko‘rinishi. Ushbu CO₂ molekulalari z o‘qi bo‘ylab bir-biridan 1,3 nm masofada joylashtirilgan. (c) [EMIM], [DCA] va [SCN] molekulalarining optimallashtirilgan tuzilmalari. CO₂ molekulalari z o‘qi bo‘ylab taxminan 1,3 nm oraliqda joylashtirilgan.

Mazkur bobda, shuningdek, gaz-ion suyuqlik qatlamli tizimlarini yaratish, ion suyuqliklar va gaz molekulalari uchun kuch maydoni parametrlarini tanlash, simulyatsiya qutilari geometriyasi, vakuum fazasi va gaz-suyuqlik interfeysi modeli tavsiflangan. [EMIM][SCN], [EMIM][DCA], [BMIM][SCN] va [BMIM][DCA]

ion suyuqliklari uchun molekulyar modellar tayyorlangan, CO_2 , H_2S va CH_4 gaz molekulalarining ion suyuqlik interfeysi orqali hajmiy fazaga o'tishini o'rganish uchun mos hisoblash tizimlari shakllantirilgan (1-rasm).

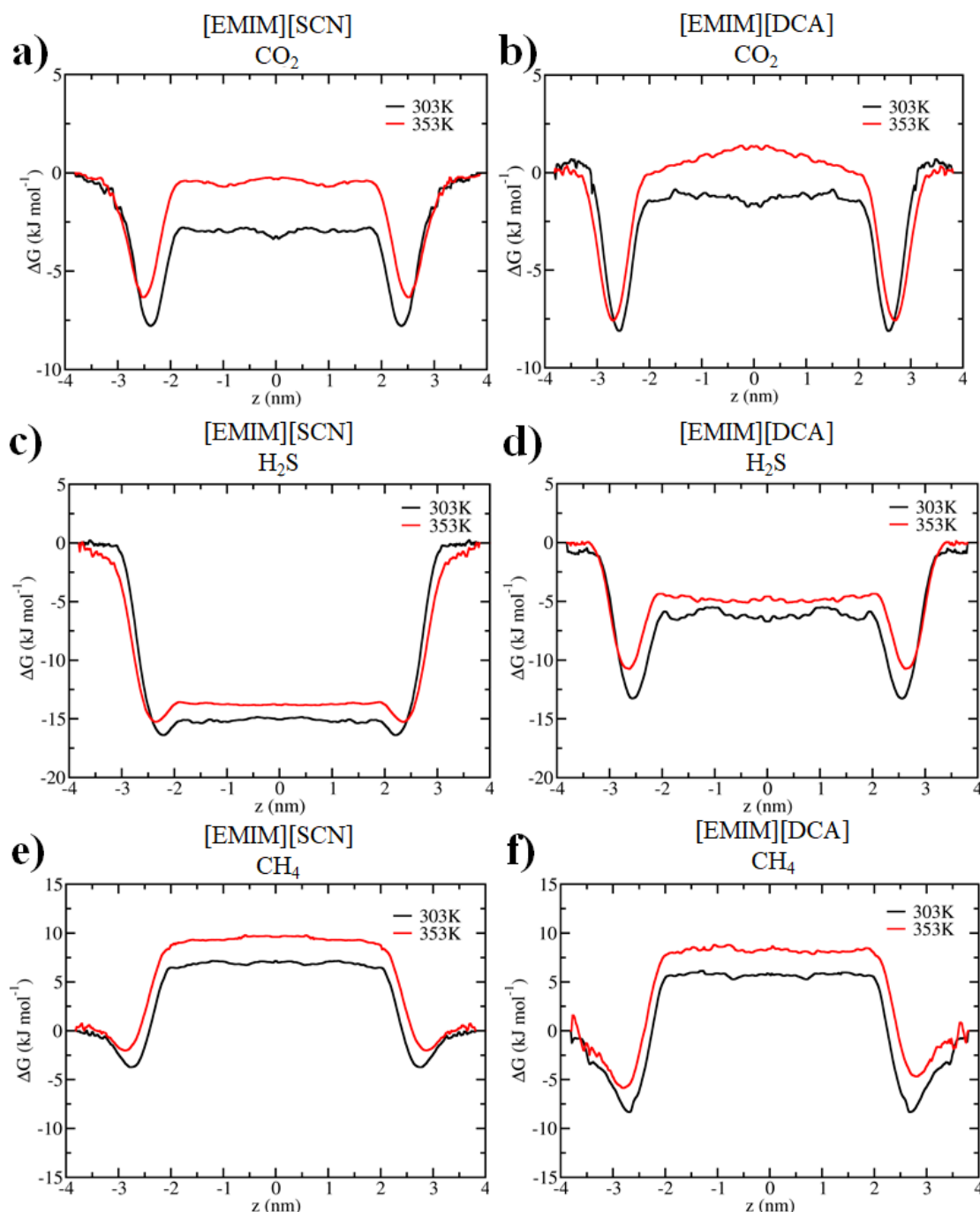
Ikkinchi bobda, shuningdek, soyabonli namunalash usuli yordamida potensial o'rtacha kuch profillarini hisoblash metodikasi ham yoritilgan. Reaksiya koordinatasi sifatida gaz molekulasining vakuumdan ion suyuqlik hajmiy fazasiga qarab interfeys-normal yo'nalishdagi harakati tanlangan. Har bir gaz molekulasi uchun erkin energiya profillari VGQAU orqali aniqlangan. Bundan tashqari, gaz zichlik taqsimoti profillari, radial taqsimot funksiyasi va diffuziya koeffitsiyentlarini hisoblash tartibi keltirilgan.

Dissertatsiyaning "[EMIM][SCN] va [EMIM][DCA] ion suyuqliklarida CO_2 , H_2S va CH_4 gazlarining yutilish xususiyatlari" deb nomlangan uchinchi bobida gazlarning termodinamik, strukturaviy va transport xususiyatlari 298, 303, 353 va 373 K haroratlarda molekulyar dinamika usullari yordamida qiyosiy tahlil qilingan. Erkin energiya profillari gaz molekulalarining interfeysda barqarorlashishi va hajmiy fazaga o'tishi gaz turi, anion tabiati hamda haroratga bog'liq ekanligini ko'rsatgan.



2-rasm. [EMIM][SCN] va [EMIM][DCA] ionli suyuqliklarida CO_2 (a,b), H_2S (c,d) va CH_4 (e,f) molekulalarining 298 K va 373 K haroratlardagi erkin energiya profillari.

CO₂ uchun ikkala ion suyuqlikda ham interfeysda manfiy erkin energiya minimumlari kuzatilgan. 298 K da interfeys erkin energiyasi [EMIM][SCN] uchun -7.6 kJ·mol⁻¹, [EMIM][DCA] uchun esa -7.7 kJ·mol⁻¹ ni tashkil etgan. Hajmiy fazada erkin energiya qiymatlari -3,1 va -2,5 kJ·mol⁻¹ ga teng bo'lgan. Harorat oshishi bilan CO₂ ning hajmiy fazadagi barqarorlashuvi, umuman olganda, kamaygan. Ushbu natijalar CO₂ ning 298 K da ikkala ion suyuqlikda ham interfeys va hajmiy fazada termodinamik jihatdan qulay barqarorlashishini ko'rsatdi.

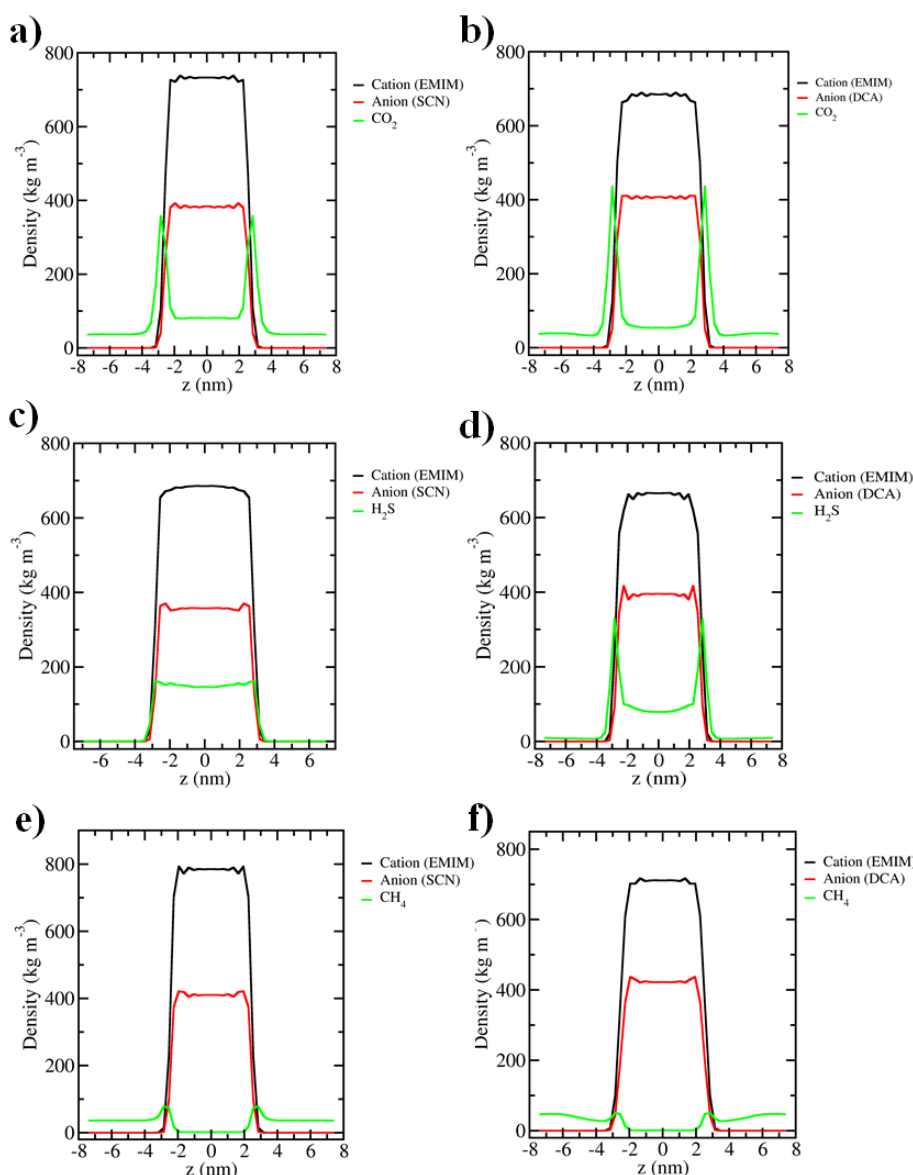


3-rasm. CO₂, H₂S va CH₄ molekularining [EMIM][SCN] va [EMIM][DCA] ion suyuqliklaridagi 303 K va 353 K haroratlardagi erkin energiya profilari.

H₂S o'rganilgan gazlar orasida eng qulay termodinamik xususiyatlarni namoyon etgan. 298 K da [EMIM][SCN] tizimida H₂S ning interfeys va hajmiy fazadagi erkin energiya qiymatlari mos ravishda -16,3 va -14,9 kJ·mol⁻¹ ni tashkil

etgan. Ushbu tizimdagi interfeysdan hajmiy fazaga o'tish energiya to'sig'i $1,4 \text{ kJ}\cdot\text{mol}^{-1}$ bo'lib, H_2S ning hajmiy fazaga o'tishi termodinamik jihatdan qulay ekanligini ko'rsatgan. $[\text{EMIM}][\text{DCA}]$ da H_2S interfeysda kuchli barqarorlashgan bo'lsa-da, hajmiy fazadagi barqarorlashuvi $[\text{EMIM}][\text{SCN}]$ ga nisbatan zaifroq bo'lgan.

CH_4 ikkala ion suyuqlikda ham interfeysda kuchsiz manfiy minimumlarga ega bo'lgan, biroq hajmiy fazadagi erkin energiya qiymatlari barcha o'rganilgan haroratlarda musbat bo'lgan. Interfeysdan hajmiy fazaga o'tish energiya to'siqlari $10 \text{ kJ}\cdot\text{mol}^{-1}$ dan yuqori bo'lib, eng katta qiymat 303 K da $[\text{EMIM}][\text{DCA}]$ tizimida $14,7 \text{ kJ}\cdot\text{mol}^{-1}$ ni tashkil etgan. Bu natijalar CH_4 ning ion suyuqlik hajmiy fazasiga o'tishi termodinamik jihatdan noqulay ekanligini ko'rsatgan.

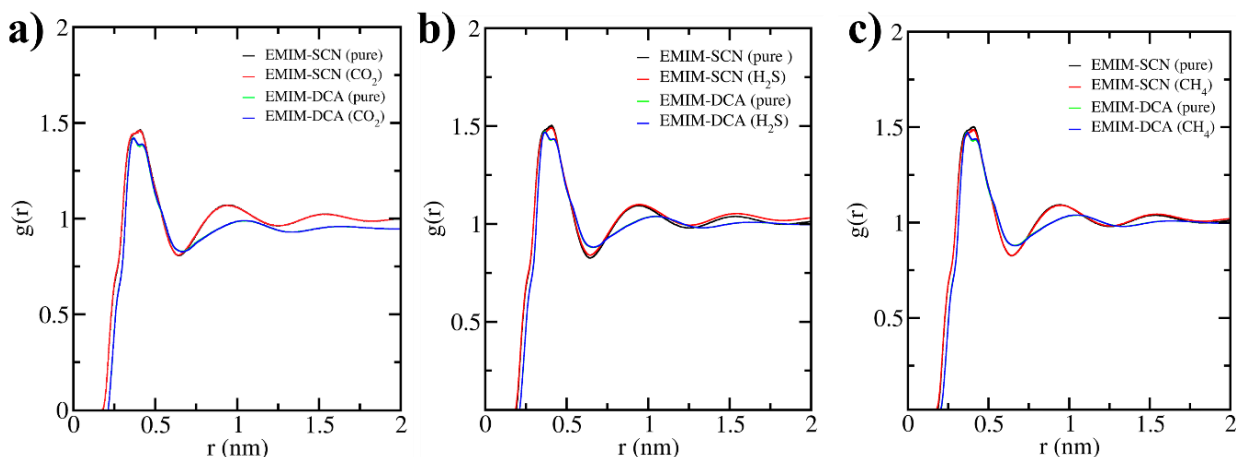


4-rasm. CO_2 , H_2S va CH_4 molekulalarining ion suyuqliklarda z o'qi bo'ylab zichlik taqsimot profillari.

Zichlik profillari CO_2 ning asosan gaz-ion suyuqlik interfeysida to'planishini, H_2S ning, ayniqsa SCN^- asosidagi tizimlarda, hajmiy fazaga chuqurroq kirishini,

CH₄ ning esa ko‘proq gaz fazasi va interfeys yaqinida taqsimlanishini ko‘rsatgan (4-rasmga qarang).

Radial taqsimot funksiyasi tahlili [EMIM][SCN] va [EMIM][DCA] ion suyuqliklarida kation-anion juftliklarining lokal strukturaviy tashkil topishini baholash uchun qo‘llanilgan. CO₂, H₂S va CH₄ molekulari kiritilganda kation-anion RDF larining asosiy maksimumlari joylashuvda sezilarli siljish kuzatilmagan, bu esa gazlarning mavjudligi ion suyuqliklarning asosiy qisqa masofali kation-anion tuzilishini sezilarli darajada buzmasligini ko‘rsatgan (5-rasmga qarang).



5-rasm. 298 K da sof va gaz molekulari mavjud [EMIM][SCN] hamda [EMIM][DCA] tizimlarida EMIM⁺ kationlari bilan SCN⁻ yoki DCA⁻ anionlari orasidagi radial taqsimot funksiyalari, g(r): (a) CO₂, (b) H₂S va (c) CH₄.

1-jadval.

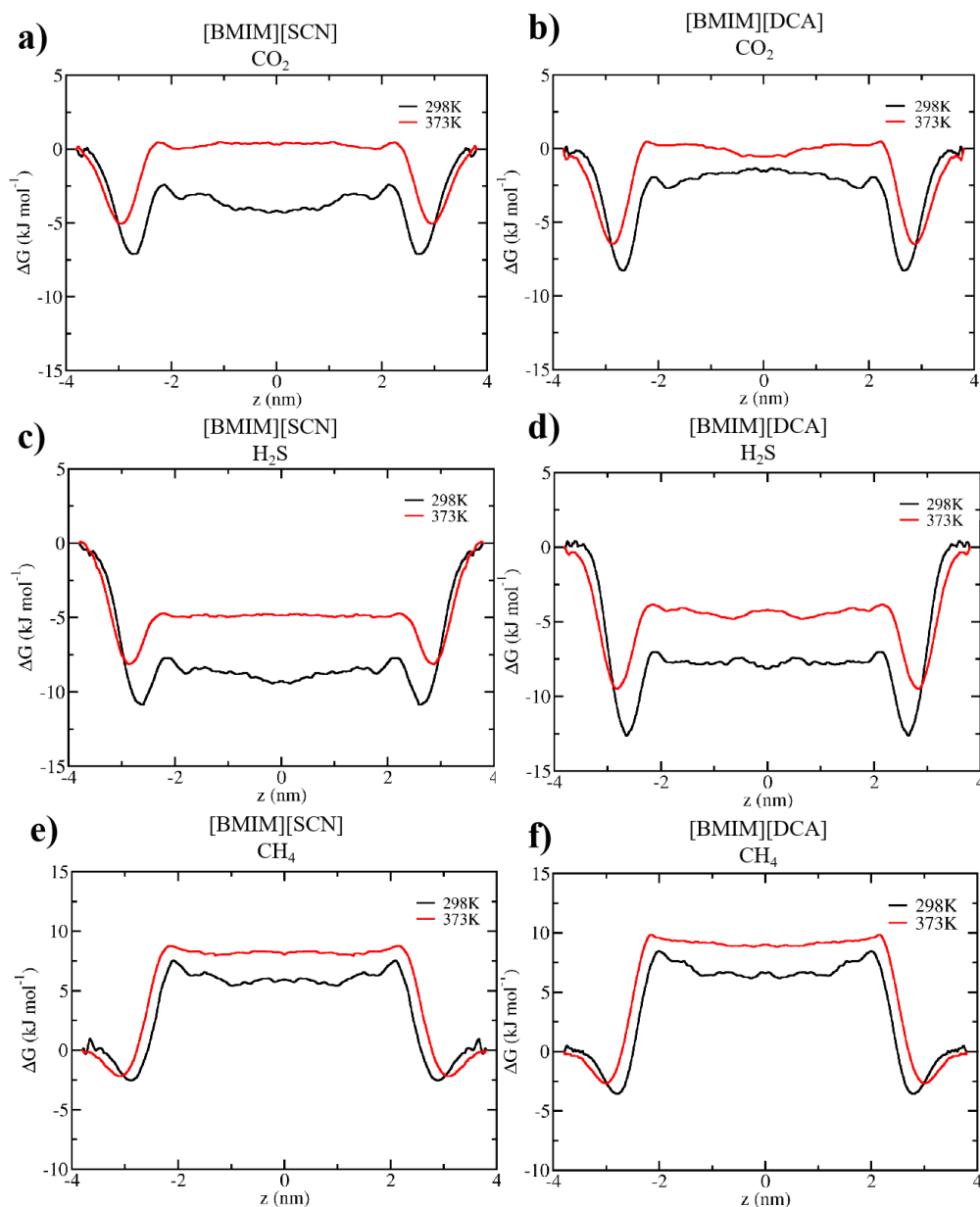
CO₂, H₂S va CH₄ molekularining [EMIM][SCN] va [EMIM][DCA] ion suyuqliklaridagi diffuziya koeffitsiyentlari.

Ion Suyuqlik	$D \times 10^{-5} \text{ cm}^2 \cdot \text{s}^{-1}$					
	CO ₂		H ₂ S		CH ₄	
	298K	373K	298K	373K	298K	373K
[EMIM][SCN]	0.2519 ± 0.003	0.9430 ± 0.001	0.2249 ± 0.004	1.1904 ± 0.002	0.4000 ± 0.002	1.2460 ± 0.001
[EMIM][DCA]	0.4743 ± 0.004	1.9327 ± 0.005	0.2768 ± 0.002	1.9625 ± 0.003	0.9700 ± 0.006	2.7800 ± 0.004

Shuningdek, uchinchi bobda CO₂, H₂S va CH₄ molekularining [EMIM][SCN] va [EMIM][DCA] dagi diffuziya koeffitsiyentlari hisoblangan (1-jadval). Harorat oshishi bilan barcha gazlar uchun diffuziya koeffitsiyentlari ortishi aniqlangan. CH₄ umuman olganda, eng yuqori molekulyar harakatchanlikni namoyon etgan. CO₂ va H₂S ning nisbiy diffuziyasi esa anion turi, gaz-anion o‘zaro

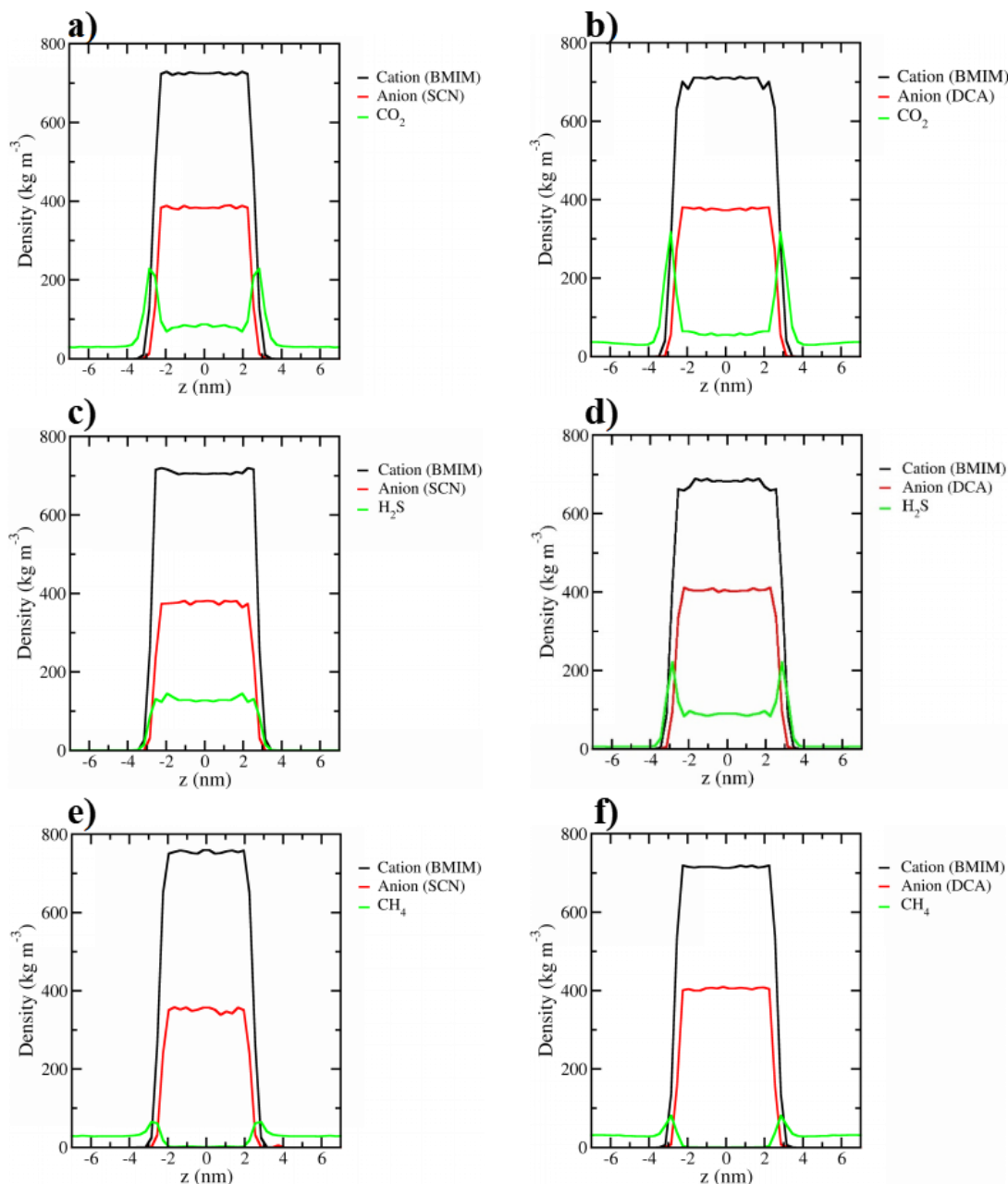
ta'siri va haroratga bog'liq holda o'zgargan. Eng katta diffuziya koeffitsiyenti 373 K da [EMIM][DCA] tizimidagi CH₄ uchun $2,78 \times 10^{-5} \text{ cm}^2 \cdot \text{s}^{-1}$ ni tashkil etgan.

Dissertatsiyaning "[BMIM][SCN] va [BMIM][DCA] ion suyuqliklarida CO₂, H₂S va CH₄ gazlarining yutilishi va transport xususiyatlari" deb nomlangan to'rtinchi bobida gazlarning erkin energiya profillari, zichlik taqsimotlari, radial taqsimot funksiyalari va diffuziya koeffitsiyentlari 298 va 373 K haroratlarda tahlil qilingan. Olingan natijalar [EMIM] asosidagi tizimlar bilan qiyoslanib, kation alkil zanjiri uzunligining ta'siri baholangan.



6-rasm. [BMIM][SCN] va [BMIM][DCA] ionli suyuqliklarida CO₂, H₂S va CH₄ molekulalarining erkin energiya profillari (FEP): (a) va (b) - CO₂ uchun [BMIM][SCN] va [BMIM][DCA]; (c) va (d) - H₂S uchun [BMIM][SCN] va [BMIM][DCA]; (e) va (f) - CH₄ uchun [BMIM][SCN] va [BMIM][DCA].

298 K da CO_2 ning interfeys erkin energiya minimumlari [BMIM][SCN] da $-7.4 \text{ kJ}\cdot\text{mol}^{-1}$ va [BMIM][DCA] da $-8,0 \text{ kJ}\cdot\text{mol}^{-1}$ ni tashkil etgan. Hajmiy fazadagi qiymatlar mos ravishda -2.45 va $-1.5 \text{ kJ}\cdot\text{mol}^{-1}$ bo'lgan. Interfeysdan hajmiy fazaga o'tish energiya to'siqlari [BMIM][SCN] va [BMIM][DCA] tizimlarida mos ravishda 4.9 va $6.5 \text{ kJ}\cdot\text{mol}^{-1}$ ni tashkil etgan. 373 K da hajmiy fazadagi erkin energiya qiymatlari nolga yaqinlashib, [BMIM][SCN] va [BMIM][DCA] da $0.5 \text{ kJ}\cdot\text{mol}^{-1}$ bo'lgan.



7-rasm. CO_2 , H_2S va CH_4 molekularining [BMIM][SCN] va [BMIM][DCA] ion suyuqliklaridagi zichlik profillari.

H_2S o'rganilgan [BMIM] tizimlarida ham CO_2 va CH_4 ga nisbatan qulayroq termodinamik xususiyatlarni namoyon etgan. 298 K da interfeys erkin energiyasi [BMIM][SCN] da $-11.2 \text{ kJ}\cdot\text{mol}^{-1}$, [BMIM][DCA] da esa $-12.7 \text{ kJ}\cdot\text{mol}^{-1}$ bo'lgan. Hajmiy fazadagi qiymatlar mos ravishda -7.6 va taxminan $-7.0 \text{ kJ}\cdot\text{mol}^{-1}$ ni tashkil

etgan. Interfeysdan hajmiy fazaga o'tish energiya to'siqlari [BMIM][SCN] da $3.6 \text{ kJ}\cdot\text{mol}^{-1}$, [BMIM][DCA] da esa $5.7 \text{ kJ}\cdot\text{mol}^{-1}$ bo'lgan.

CH_4 ning hajmiy fazadagi erkin energiya qiymatlari ikkala ion suyuqlikda ham musbat bo'lgan. 298 K da interfeysdan hajmiy fazaga o'tish energiya to'siqlari [BMIM][SCN] da $10.2 \text{ kJ}\cdot\text{mol}^{-1}$ va [BMIM][DCA] da $11.3 \text{ kJ}\cdot\text{mol}^{-1}$ ni tashkil etgan. Bu holat CH_4 ning hajmiy fazaga o'tishi termodinamik jihatdan noqulay ekanligini ko'rsatgan.

Zichlik profillari CO_2 va H_2S ning interfeysga moyilligini, H_2S ning ayrim tizimlarda hajmiy fazaga chuqurroq kirishini, CH_4 ning esa asosan gaz fazasi va interfeys yaqinida taqsimlanishini ko'rsatgan. Radial taqsimot funksiyalari SCN^- va DCA^- anionlarining gaz molekullari bilan turlicha lokal strukturaviy korrelatsiyalar hosil qilishini aniqlash imkonini bergan.

Diffuziya koeffitsiyentlari barcha gazlar uchun harorat oshishi bilan sezilarli ortgan. 298 K da CH_4 ning diffuziya koeffitsiyenti [BMIM][SCN] da $0.190 \times 10^{-5} \text{ cm}^2\cdot\text{s}^{-1}$ va [BMIM][DCA] da $0.438 \times 10^{-5} \text{ cm}^2\cdot\text{s}^{-1}$ bo'lgan. 373 K da ushbu qiymatlar mos ravishda 1.261×10^{-5} va $1.770 \times 10^{-5} \text{ cm}^2\cdot\text{s}^{-1}$ ga yetgan. [EMIM]⁺ dan [BMIM]⁺ ga o'tish gazlarning umumiy termodinamik afzallik tartibini o'zgartirmagan, biroq ularning molekulyar harakatchanligini, umuman olganda, kamaytirgan.

Umuman olganda, to'rtinchi bob natijalari [EMIM] dan [BMIM] ga o'tish gaz yutilishining umumiy tartibini tubdan o'zgartirmasligini ko'rsatgan. H_2S eng qulay yutiluvchi gaz, CO_2 o'rtacha yutiluvchi gaz, CH_4 esa hajmiy fazaga kirishi noqulay gaz sifatida namoyon bo'lgan. Kation alkil zanjiri uzunligining ta'siri asosan diffuziya, hajmiy fazadagi gaz joylashuviga bog'liq bo'lib, gaz selektivligini belgilashda anion asosiy rol o'ynashi aniqlangan.

2-jadval.

CO_2 , H_2S va CH_4 molekullarining [BMIM][SCN] va [BMIM][DCA] ion suyuqliklaridagi diffuziya koeffitsiyentlari.

Ion suyuqlik	$D \times 10^{-5} \text{ cm}^2\cdot\text{s}^{-1}$					
	CO_2		H_2S		CH_4	
	298 K	373 K	298 K	373 K	298 K	373 K
[BMIM][SCN]	0.137	0.675	0.147	0.766	0.190	1.261
	± 0.002	± 0.002	± 0.004	± 0.007	± 0.005	± 0.004
[BMIM][DCA]	0.151	0.827	0.215	0.795	0.438	1.770
	± 0.001	± 0.005	± 0.001	± 0.007	± 0.003	± 0.001

XULOSA

1. [EMIM][SCN], [EMIM][DCA], [BMIM][SCN] va [BMIM][DCA] ion suyuqliklarining molekulyar modellari uchun hisoblangan zichlik qiymatlarining mavjud tajribaviy ma'lumotlar bilan yaxshi mos kelishi tanlangan kuch maydoni parametrlarining gaz-ion suyuqlik tizimlarini modellashtirish uchun ishonchliligini ko'rsatdi.

2. CO₂, H₂S va CH₄ gazlarining vakuumdan ion suyuqlik hajmiy fazasiga o'tish erkin energiya profillari aniqlanib, H₂S o'rganilgan gazlar orasida eng qulay termodinamik yutilishni namoyon qilishi aniqlandi. 298 K da [EMIM][SCN] tizimida H₂S ning interfeys va hajmiy fazadagi erkin energiya qiymatlari mos ravishda -16,3 va -14,9 kJ·mol⁻¹, interfeysdan hajmiy fazaga o'tish energetik to'sig'i esa 1,4 kJ·mol⁻¹ ni tashkil etdi.

3. CO₂ ning barcha o'rganilgan ion suyuqliklarda hajmiy fazaga nisbatan interfeysda kuchliroq barqarorlashishi aniqlandi. 298 K da eng kichik interfeys erkin energiya minimumi [BMIM][DCA] tizimida -8,0 kJ·mol⁻¹ ni tashkil etdi. DCA⁻ asosidagi ion suyuqliklarda CO₂ ning interfeysda barqarorlashishi SCN⁻ asosidagi tizimlarga nisbatan kuchliroq ekanligi aniqlandi.

4. CH₄ ning hajmiy fazaga o'tishi barcha o'rganilgan ion suyuqliklarda termodinamik jihatdan noqulay ekanligi aniqlandi. Uning hajmiy fazadagi erkin energiya qiymatlari barcha tekshirilgan haroratlarda musbat bo'lib, interfeysdan hajmiy fazaga o'tish energetik to'siqlari 10 kJ·mol⁻¹ dan yuqori bo'ldi. Bu natijalar o'rganilgan ion suyuqliklarda H₂S va CO₂ ning CH₄ ga nisbatan termodinamik afzalligini ko'rsatdi.

5. Zichlik taqsimoti tahlili erkin energiya natijalarini tasdiqlab, CO₂ ning asosan gaz-ion suyuqlik interfeysida to'planishi, H₂S ning, ayniqsa SCN⁻ asosidagi tizimlarda, hajmiy fazaga chuqurroq kirishi, CH₄ ning esa asosan interfeys va vakuum sohasi yaqinida taqsimlanishi aniqlandi.

6. CO₂, H₂S va CH₄ gazlarining molekulyar diffuziyasi harorat va ion suyuqlik tuzilishiga sezilarli bog'liq ekanligi aniqlandi. Harorat 298 K dan 373 K gacha oshirilganda barcha gazlarning diffuziya koeffitsiyentlari ortdi, DCA⁻ asosidagi ion suyuqliklarda esa ular, umuman olganda, mos SCN⁻ tizimlariga qaraganda yuqoriroq bo'ldi. Eng yuqori diffuziya koeffitsiyenti 373 K da [EMIM][DCA] tizimidagi CH₄ uchun $2.78 \times 10^{-5} \text{ cm}^2 \cdot \text{s}^{-1}$ ni tashkil etdi.

7. Olingan termodinamik, strukturaviy va transport natijalari asosida SCN⁻ asosidagi ion suyuqliklar H₂S ning hajmiy fazaga o'tishi uchun, DCA⁻ asosidagi tizimlar esa CO₂ ning interfeysda barqarorlashishi va gazlarning yuqoriroq molekulyar harakatchanligi uchun nisbatan qulay ekanligi aniqlandi. Ushbu natijalar CO₂ va H₂S ni CH₄ dan ajratishga mo'ljallangan ion suyuqliklarni dastlabki

molekulyar saralash va tabiiy gazni tozalash uchun istiqbolli tizimlarni baholashga ilmiy-uslubiy asos yaratdi.

**НАУЧНЫЙ СОВЕТ DSc.03/06.11.2025.K/FM.10.09 ПРИ ИНСТИТУТЕ
ФУНДАМЕНТАЛЬНЫХ И ПРИКЛАДНЫХ ИССЛЕДОВАНИЙ ПО
ПРИСУЖДЕНИЮ УЧЁНОЙ СТЕПЕНИ**

**ИНСТИТУТ ФУНДАМЕНТАЛЬНЫХ И ПРИКЛАДНЫХ
ИССЛЕДОВАНИЙ**

ҚОДИРОВ АКБАР ИСМОИЛ ЎҒЛИ

**ИССЛЕДОВАНИЕ АБСОРБЦИИ ГАЗОВ CO₂, H₂S И CH₄ В ИОННЫХ
ЖИДКОСТЯХ НА ОСНОВЕ ПРОИЗВОДНЫХ ИМИДАЗОЛА
МЕТОДАМИ МОЛЕКУЛЯРНОЙ ДИНАМИКИ**

02.00.04 - Физическая химия

АВТОРЕФЕРАТ ДИССЕРТАЦИИ ДОКТОРА ФИЛОСОФИИ (PhD)

Ташкент-2026

Тема диссертации доктора философии (PhD) по физико-математическим наукам зарегистрирована в Высшей аттестационной комиссии при Министерстве высшего образования, науки и инноваций Республики Узбекистан за номером B2026.2.PhD/FM1550.

Диссертация выполнена в Институте фундаментальных и прикладных исследований.

Автореферат диссертации на трёх языках (узбекский, английский, русский (резюме)) размещён на веб-странице по адресу www.ifar.uz и на Информационно-образовательном портале «Ziynet» по адресу www.ziynet.uz

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Защита диссертации состоится “___” _____ 2026 года в ___ часов на заседании Научного совета DSc.03/06.11.2025.K/FM.10.09 при Институте фундаментальных и прикладных исследований (Адрес: 100000, Ташкент, ул. Кори Ниёзи, 39А, тел.: (+99871) 237-09-61, факс: (+99871) 237-09-61, e-mail: info@ifar.uz).

С диссертацией можно ознакомиться в Информационно-ресурсном центре Института фундаментальных и прикладных исследований (Зарегистрировано под № ____). Адрес: 100000, Ташкент, ул. Кори Ниёзи, 39А, тел.: (+99871) 237-09-61, факс: (+99871) 237-09-61.

Автореферат диссертации разослан «___» _____ 2026 года.

(реестр протокола рассылки № ____ от «___» _____ 2026 года).

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ВВЕДЕНИЕ (аннотация диссертации доктора философии (PhD))

Целью исследования является определение механизмов поглощения и транспорта диоксида углерода, сероводорода и метана в циано-функционализированных ионных жидкостях на основе имидазолия методами молекулярной динамики.

Научная новизна исследования заключается в следующем:

определены профили свободной энергии переноса молекул CO_2 , H_2S и CH_4 из вакуумной области через границу раздела газ–ионная жидкость в объёмную фазу циано-функционализированных ионных жидкостей на основе имидазолия [EMIM][SCN], [EMIM][DCA], [BMIM][SCN] и [BMIM][DCA];

установлен общий порядок термодинамического предпочтения исследованных газов в ионных жидкостях: $\text{H}_2\text{S} > \text{CO}_2 > \text{CH}_4$; выявлено, что молекулы H_2S более устойчиво стабилизируются в объёмной фазе, тогда как молекулы CO_2 преимущественно стабилизируются на границе раздела газ–ионная жидкость;

определены энергетические барьеры перехода молекул CO_2 , H_2S и CH_4 от границы раздела в объёмную фазу и установлена их зависимость от природы газа, типа аниона и температуры; выявлено, что переход H_2S в объёмную фазу является более благоприятным в ионных жидкостях на основе SCN^- , тогда как переход CH_4 в объёмную фазу термодинамически неблагоприятен во всех исследованных системах;

установлены закономерности пространственного распределения молекул газов в ионных жидкостях в зависимости от природы аниона: CO_2 преимущественно накапливается на границе раздела в системах с обоими типами анионов; H_2S относительно более равномерно распределяется в объёмной фазе систем на основе SCN^- , тогда как в системах на основе DCA^- преимущественно накапливается на границе раздела; CH_4 преимущественно накапливается на границе раздела;

установлено, что увеличение длины алкильной цепи катиона от [EMIM]⁺ до [BMIM]⁺ не изменяет общий порядок термодинамического предпочтения газов, но приводит к снижению коэффициентов их молекулярной диффузии; также выявлено, что молекулярная подвижность газов в ионных жидкостях на основе DCA^- выше, чем в соответствующих системах на основе SCN^- .

Внедрение результатов исследования:

Результаты молекулярно-динамического исследования поглощения и транспорта CO_2 , H_2S и CH_4 в ионных жидкостях на основе имидазолия были использованы в научно-исследовательской деятельности Исследовательского центра по улавливанию и использованию диоксида углерода (Research Centre for Carbon Dioxide Capture and Utilisation, CCDCU) Университета Sunway, Малайзия, что официально подтверждено 15 августа 2025 года.

Кроме того, статья, опубликованная по результатам исследования в международном научном журнале, индексируемом в базе Scopus, была процитирована 8 раз, что свидетельствует о научной значимости и признании полученных результатов международным научным сообществом.

Структура и объём диссертации:

Диссертация состоит из введения, четырёх глав, заключения, списка использованной литературы и приложений. Общий объём диссертации составляет 120 страниц.

E'LON QILINGAN ISHLAR RO'YXATI
LIST OF PUBLISHED WORKS
СПИСОК ОПУБЛИКОВАННЫХ РАБОТ

I bo'lim (I часть; I part)

1. Kodirov A., Abduvokhidov D., Mamatkulov Sh., Shahzad A., Razzokov J. The Absorption Mechanisms of CO₂, H₂S and CH₄ Molecules in [EMIM][SCN] and [EMIM][DCA] Ionic Liquids: A Computational Insight // Fluid Phase Equilibria. - 2024. - Vol. 581. - Article 114080.
2. Kodirov A., Aroua M.K., Razzokov J. Permeation behavior of CO₂, H₂S, and CH₄ in imidazolium-based ionic liquids: A molecular dynamics study // Computational and Theoretical Chemistry. - 2025. - Vol. 1253. - Article 115446.
3. Kodirov A., Razzokov J. Free energy analysis of CO₂, H₂S, and CH₄ in cyano-functionalized ionic liquids: effect of temperature and anion structure // Development of Science. - 2026. - Vol. 4, №3.
4. Kodirov A., Razzokov J. Gas transport and structural effects in [EMIM][SCN] and [EMIM][DCA] ionic liquids: a molecular dynamics study // Development of Science. - 2026. - Vol. 7, №3.

II bo'lim (II часть; II part)

1. Kodirov A., Razzokov J. The Absorption Mechanisms of CO₂, H₂S and CH₄ Molecules in EMIMBF₄ and EMIMDCA Ionic Liquids // “Ta’lim, fan va ishlab chiqarishning dolzarb muammolari” mavzusidagi respublika ilmiy-amaliy konferensiya materiallari to‘plami. - Namangan: Namangan muhandislik-texnologiya instituti, 7-8-noyabr, 2023. - B. 310-313.
2. Kodirov A., Shukurov O., Rasulov Sh., Razzokov J. Permeation Dynamics of CO₂, H₂S, and CH₄ in BMIMTCM Ionic Liquid: A Molecular Dynamics Study // “Fizikaning zamonaviy muammolari va rivojlanish istiqbollari” I xalqaro ilmiy-amaliy konferensiya materiallari to‘plami. - Namangan, 22-23-oktabr, 2024. - B. 409-410.
3. Kodirov A., Razzokov J. Interfacial and bulk diffusion of CO₂, H₂S, and CH₄ in [BMIM][SCN]: A computational study // Proceedings of Abstracts of the International Conference “New Materials and Solar Technologies”. - Parkent, Uzbekistan, 28-30 April, 2025. - P. 71-72.
4. Kodirov A., Razzokov J. Molecular-level understanding of CO₂ adsorption in [BMIM][TCM] ionic liquid // “Fan va ishlab chiqarish sohalarida zamonaviy fizik-kimyoviy tadqiqot usullari integratsiyasi” mavzusidagi xalqaro olimlar ishtirokidagi ilmiy-amaliy anjuman materiallari to‘plami. - Toshkent-Urganch, 17-18-oktabr, 2025. - B. 95-96.

Avtoreferat “Fan va innovatsiyalar” xalqaro ilmiy jurnali (International scientific journal “Science and Innovation”) tahririyatida tahrirdan o‘tkazilib, o‘zbek, va rus tillaridagi matnlari o'zaro muvofiqlashtirildi (03.10.2026 yil).



Bosishga ruxsat etildi: 03.10.2026-yil.
Bichimi 60x84^{1/16}, “Times New Roman”
garniturada raqamli bosma usulida bosildi.
Shartli bosma tabog‘i 2,7. Adadi: 100. Buyurtma: № 134.
Tel (99) 817 44 54.
Guvohnoma reyestr № 219951
“PUBLISHING HIGH FUTURE” OK nashriyotida bosildi.
Toshkent sh., Uchtepa tumani, Ali Qushchi ko‘chasi, 2A-uy.