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Molecular Dynamics Study of Carbon Dioxide Gas Within Ice XVII Structure

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Abstract: We conducted a molecular dynamics study on CO_2 hydrate within the ice XVII structure to examine the molecular diffusion of CO_2 molecules, as it is essential to the hydrate potential as a carbon capture. The simulated CO_2 hydrate system used 324 water molecules and 90 CO_2 molecules. We used the TIP4P/Ice model for water molecules, and the CO_2 molecules were treated as united atom. The simulations were carried out at 273,15 K under various pressures of 200 MPa, 500 MPa, and 1000 MPa for 1,50 ns, with a step size of 1 fs. The results showed that the CO_2 molecules were confined and freely moved inside the cage-like chiral tube along the c-axis of the ice XVII structure. No significant inter-cage hopping was observed during the evolution of all simulated systems. The diffusion coefficient values for CO_2 molecules within the ice XVII structure were 5.03×10^{-8} cm^{2}s^{-1}, 2.45×10^{-8} cm^{2}s^{-1}, and 8.86×10^{-8} cm^{2}s^{-1} for the respective pressure variations of 200 MPa, 500 MPa, and 1000 MPa, resulting in an inverse proportional with the system's pressure. A higher diffusion coefficient facilitates a faster the mass transfer and adsorption rate of CO_2 in formation build up of the CO_2 hydrate system.

Keywords: CO_2 hydrate; Diffusion coefficient; Ice XVII; Molecular dynamics

Introduction

Solid inclusion compounds known as hydrates have structures similar to ice. They are created by encapsulating hydrophobic gas molecules within a framework of hydrogen-bonded water molecules under specific temperature and pressure conditions (Xu et al., 2022). The hydrogen-bonded water molecules form cage-like structures capable of trapping gas molecules. Hydrates are generally divided into clathrates and filled ice (Hassanpouryouzband et al., 2020; Hirai & Kadobayashi, 2023). Hydrates present a promising solution for improving food preservation (Pandey et al., 2024), the effective storage of energy source gases (Del Rosso et al., 2017; Kuhs et al., 2018; Chen et al., 2019 Gambelli et al., 2022; Dewangan et al., 2022; Saikia et al., 2023; Kim & Ahn, 2024), and the mitigation of environmental challenges, including the accumulation of carbon dioxide (Liang et al., 2016; Zhou et al., 2021). This potential represents a valuable addition to previously developed carbon capture methods (Field & Mach, 2017; Xia et al., 2019; Wang et al., 2020; Liu et al., 2022; G. Pandey et al., 2022; Verstreken et al., 2024; Yang et al., 2024).

Carbon dioxide (CO_2) hydrate is a non-stoichiometric crystalline compound that can host CO_2 molecules in its cavities. Under low pressures, CO_2 hydrate is reported to have structure I (sI) and transformed into ice VI and dry ice under high pressures (Tulk et al., 2014; Hirai & Kadobayashi, 2023). A newly observed phase of CO_2 hydrate, where its pressure is positioned between sI and ice VI-CO_2, has been reported (Hirai et al., 2010). This new structure resembles the reported hydrogen hydrate C_0 structure (del Rosso et al., 2021; Hirai & Kadobayashi, 2023). The extraction of gas molecules from the hydrate lattice under vacuum conditions leads to the formation of a metastable ice structure referred to as ice XVII (del Rosso et al., 2017),

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that transform into cubic ice Ic with high structural purity when carefully heated (del Rosso et al., 2020). Ice XVII, derived from hydrogen hydrate type C0, showcases a spiral tunnel structure with a hexagonal orientation along the z-axis, measuring 5.26 Å in length and 6.10 Å in diameter (Del Rosso, Grazzi, et al., 2016; Michl et al., 2019). The void spaces within this hydrate can accommodate gases even at pressures well below atmospheric pressure (del Rosso et al., 2017). This characteristic renders ice XVII ideal for engaging hydrophobic gases such as hydrogen and carbon dioxide. The ice XVII structured CO_2 hydrate can have a 1:3.55 ratio at low pressures and a 1:4 ratio at high-pressure regimes. Within this structure, CO_2 gas molecules are aligned along the spiral tunnels, exhibiting their confinement within the void space (Pradana et al., 2020).

This study involved molecular dynamics simulation to examine the diffusion of CO_2 molecules within the ice XVII structure, aiming to offer comprehensive molecular insights into the CO_2 hydrate system, as the hydrate system is essential for carbon capture. The study thoroughly presented the molecular mechanisms and diffusion coefficients of CO_2 gas molecules resulting from the simulations. These analytical outcomes are poised to significantly complement experimental methodologies, thereby contributing to the advancement of technologies concerning the interaction of CO_2 molecules with the ice XVII structure.

Method

This study performed a molecular dynamics calculation of CO_2 molecules within the ice XVII, to obtain the diffusion distinctive in this specific ice XVII structure of C0 hydrate. It is reported that ice XVII-based C0 is found to be stable up to 180 MPa at 308K (Michl et al., 2019). The ice XVII structure was created by utilizing 324 water molecules arranged in a 3 × 3 × 3 unit cell. By introducing 90 CO_2 molecules, a CO_2 hydrate system within ice XVII at a 1:3.6 ratio was carefully created using the Genice package (Matsumoto et al., 2018). Were conducted on 3 pressure conditions, namely 200 MPa, 500 MPa, and 1000 MPa.

The equilibration process performed for 0.25 ns, followed by a production run for 1.50 ns with a time step The water molecules were modeled using the TIP4P/ice model, replicating the model setup of a previous study on filled ice II - hydrogen hydrate (Harada et al., 2019), and C2 hydrogen hydrates (Arman & Nugroho, 2021), while the carbon dioxide gas was represented as united atom located at its center of mass with parameters taken from Polat et al. (2024). The flowchart of the whole simulation processes can be seen in Figure 1. Figure 2 shows the simulated structure. CO_2 molecules are placed inside the chiral tube along the c-axis, aligned to the other CO_2 guest molecules when projected onto the ab (basal) plane as depicted in Figure 2(a). The simulations of 1 fs. Coulomb interactions were computed using the Particle-Particle Particle Mesh (PPPM) method with interaction cutoff corrections and a switching function initiated at a radius of 10 Å. The modified Verlet-rRESPA method was employed to solve the equations of motion, including thermostat and barostat variables. All molecular dynamics simulation was performed by using LAMMPS (Thompson et al., 2022).

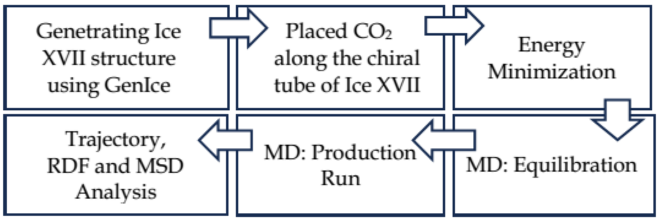

Figure 1. The flow chart of the Simulation processes

The total potential energy of the system is determined by summing the potential energies of pairwise interactions between molecules. Specifically, in this simulation, the non-bonded interactions between molecules are composed of the Lennard-Jones potential and the electrostatic potential. The system's potential energy for intermolecular interactions can be mathematically expressed through the equation (1).

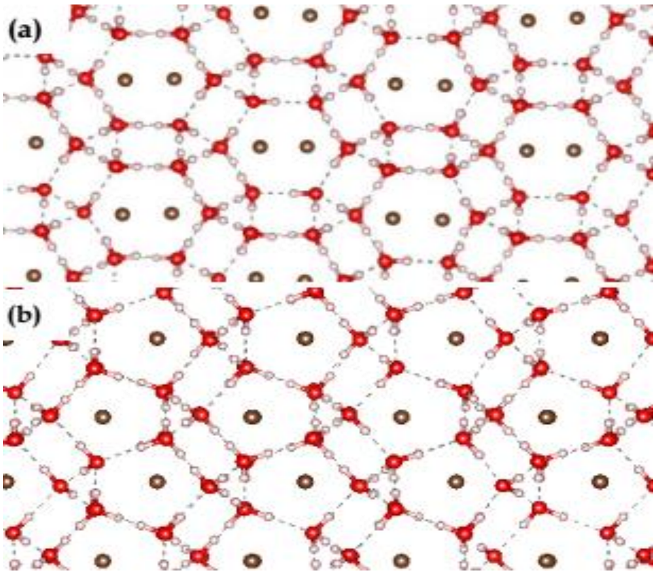

Figure 2. CO_2 hydrate structure within ice XVII with a 1:3.6 ratio is shown in (a) the *ab* plane, and (b) the *bc* plane. The brown spheres represent CO_2 gas molecules, and the combination of the red and white spheres corresponds to the hydrogen-bonded water molecule framework. This figure was created using the VESTA application (Momma & Izumi, 2008)

$$\phi = \sum_{i,j}\left[4\varepsilon_{ij}\left\{\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12}-\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right\}+\frac{q_i q_j e^2}{r_{ij}}\right] \tag{1}$$

where ε represents the minimum energy interaction (in kcal/mol), σ is the distance between molecules at which the interaction potential is at its minimum, and r denotes the distance between molecules at which the interaction potential is zero. The parameter q represents the charge of the interacting atom, while e is the magnitude of the electron charge. The parameters used in this study are listed in Table 1. The interaction between water molecules and guest molecules is characterized using the Lorentz-Berthelot mixing rules.

To analyze the diffusion of CO_2 gas molecules (D), the mean squared displacement of CO_2 molecules was calculated at each time interval using the Einstein relation (Koirala et al., 2020).

$$D = \frac{1}{6t}\langle[\boldsymbol{r_i}(t)-\boldsymbol{r_i}(0)]^2\rangle \tag{2}$$

where $r_i(t)$ is the position vector of molecule i at time t and $r_i(0)$ is its initial position. The angle brackets ⟨…⟩ in the equation denote ensemble averages. The term $\langle[r_i(t)-r_i(0)]^2\rangle$ represents the time correlation function of the position vector. The diffusion coefficient ($cm^2\ s^{-1}$) is obtained by interpolating the MSD graph as a function of time interval.

Result and Discussion

In this study, the structural configuration was analyzed using Radial Distribution Function (RDF) profiles for pairs of water molecules (O-O), water molecules with CO_2 molecules pairs (O-CO_2), and CO_2-CO_2 molecules. Figure 3 illustrates the RDF profiles for O-O pairs of water molecules forming ice XVII. Ice XVII is an ice polymorph obtained from the extraction of hydrogen gas trapped in type C0 hydrogen hydrates. This structure has a hexagonal unit cell with space group P6122 (Amos et al., 2017), which can also encapsulate Nitrogen (Liu et al., 2022; Massani et al., 2019).

The RDF graph for the O-O pairs in this structure has 4 peaks, with the fourth peak being more broadly distributed. This aligns with the RDF profile of H_2 hydrate systems in the ice XVII structure reported previously (Strobel et al., 2016; Del Rosso et al., 2017; Ikeda, 2021; Del Rosso et al., 2016).

Such patterns are indicative of typical hydrate structure characteristics. In each simulated system, the first peak of the profile is around ~2.7 Å, indicating the presence of bulk water structure encapsulating hydrophobic gas. The second peak is about ~4.5 Å and the third around ~6.5 Å, showing a diminishing trend with increasing pressure, indicating reduced void distortions caused by encapsulation mechanisms within this structure.

Table 1. The Parameters of CO_2 and TIP4P/Ice

Model	Site	q(e)	σ(Å)	ε (kcal mol^{-1})
CO_2	Center	-	3.7410	0.3869
	H	+0.5897	-	-
TIP4P/Ice	O	-	3.1688	0.2108
	M	-1.1794	-	-

The position of the first peak bears similarity to neutron diffraction study results on Ne and O_2 hydrates in ice XVII structure reported (Catti et al., 2019). When encapsulating a hydrophobic solute like CO_2, water molecules orient themselves to confine the gas molecules of CO_2 bonding environments while keeping their distance from those confined guests.

The RDF profile of all simulated systems shifts towards smaller interaction distances under higher pressure. Compared with hydrogen hydrate in the same ice structure and pressure conditions (500 MPa), the RDF O-O profile at a distance over ~8.8 Å shows significant differences. Hydrogen hydrate exhibits a sharper profile, whereas in CO_2 hydrate systems, this range is broader, approximately ~8.0 Å to ~10.0 Å, though bearing towards sharper peaks with increasing system pressure. This difference arises from the size of guest molecules: CO_2 molecules have a larger molecular size than H_2 gas molecules.

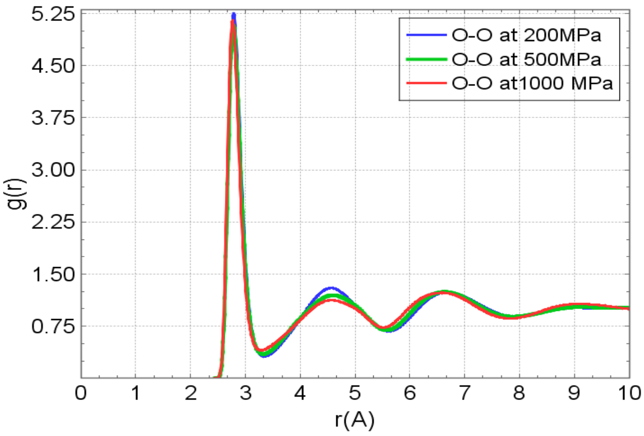

Figure 3. Radial distribution function of O-O pair interaction for all of the simulated systems

The RDF profiles for O-CO_2 and CO_2-CO_2 molecular interaction pairs are presented in Figure 3. For the O-CO_2 pairs, the RDF profile shows a narrow bell-shaped curve with 3 peaks. Similar to the O-O pairs, these peaks shift towards smaller interaction distances under higher pressures. Every peak on all simulated systems shifts by approximately ~0.2 Å from 200 MPa to

1000 MPa. At 1000 MPa, the RDF profile after the second peak becomes sharper, followed by a slight broadening.

Based on the RDF profile for CO_2-CO_2 molecular pairs, the separation distance within the filled void ranges from 3.3 Å to 5.3 Å. Increasing system pressure shows a narrowing of this range (from 3.3-4.93 Å at 1000 MPa). This indicates that the void spaces compacted under higher pressures. The peaks are asymmetric, reflecting that the CO_2 molecules do not always occupy the center of the available void. The void spaces remain sufficiently large to allow the CO_2 molecules to diffuse and oscillate. To examine the diffusion mechanism of these gas molecules, we present trajectories of CO_2 gas molecules from 0.5 ns to 1.25 ns (Figure 4).

As can be seen from Figure 4, it is evident that the CO_2 gas molecules are confined in a cage-like structure, moving randomly within the void spaces. These voids form pores that create spiral tunnels along the c-axis. As the system pressure increases, the movement of the gas molecules becomes more constrained. This is also shown by the O-CO_2 RDF profile, indicating that the cage-like tunnels shrink in volume, restricting the movement of CO_2 gas molecules. Previous studies have also stated the slower diffusion of heavier species along the spiral channel-like structure of ice XVII.

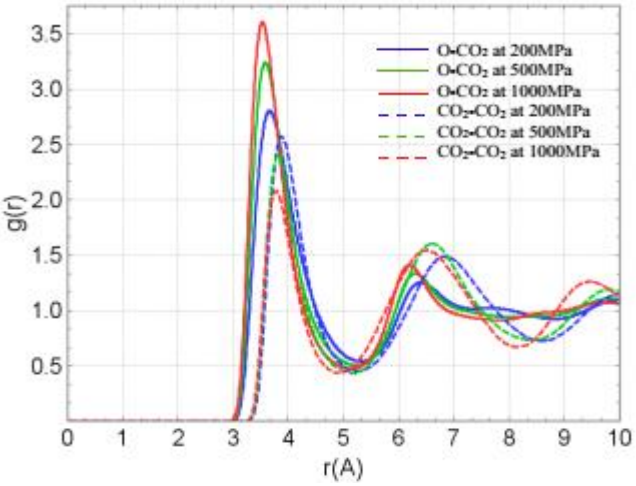

Figure 4. RDF profile of O-CO_2 pair (Colored solid lines) and CO_2-CO_2 pair (colored dashed lines). The Blue, green, and red color shows the system undergoes 200MPa, 500MPa, and 1000MPa of pressure, respectively

Understanding the molecular diffusion mechanisms within gas hydrate phases is important to enhance the hydrate formation techniques. A previous study of neutron diffraction experiments reported that CO_2 gas molecules predominantly exhibit librational motion (Ida et al., 2013; del Rosso et al., 2024). Therefore, we calculate the Mean Squared Displacement (MSD) values for CO_2 gas molecules within the ice XVII structure to get more insights into the guest-molecule diffusion inside the spiral tunnels along the c-axis.

Table 2. Diffusion Coefficient of CO_2 Inside the Ice XVII Structure

System	Pressure	D ($cm^2 s^{-1}$)
This work (C0 at 273.15 K)	500 MPa	2.45×10^{-8}
	1000 MPa	8.86×10^{-9}
Experimental results. *Structure 1 CO_2 hydrate (270 K) (Liang et al., 2016)	100 MPa	$1.00 \times 10^{-12} \sim 2.00 \times 10^{-10}$

Interpolated MSD values for each simulation time interval were used to derive diffusion coefficients, presented in Table 2. These coefficients indicate a decrease with increasing system pressure. The diffusion coefficient is at the highest (5.03×10^{-8} cm^2 s^{-1}) when systems undergo 200 MPa, supporting the RDF analysis of the CO_2 hydrate structure, which suggests that shrinking void sizes limit the movement of CO_2 gas molecules. The confinement of CO_2 gas molecules by a chain of hydrogen-bonded water molecules is also expected to decrease the diffusion coefficient. This is due to the preferential adsorption and steric hindrance that may contribute further to the reduction in diffusion (Polat et al., 2024).

When comparing the diffusion coefficient of CO_2 in the S1 structure and the ice XVII structure which has the same potential as carbon capture, we find that the diffusion coefficient of CO_2 in the ice XVII structure is higher. In the ice XVII structure, CO_2 gas molecules can move along the chiral tunnels along the c-axis. On the other hand, the S1 structure includes two types of cages (5^{12} and $5^{12}6^2$) with significant energy barriers. It's worth noting that the calculated diffusion coefficient is inversely related to the system pressure. This corresponds to the kinetic theory of gases, which states that the average kinetic energy of molecules in a closed system is inversely proportional to the system pressure, as mentioned earlier. The increasing density of hydrate system limits the movement of CO_2 inside the cage.

The diffusion coefficient is crucial in the process of CO_2 hydrates buildup, and the implementation of various technologies, including carbon capture. Hydrates form when water molecules create cage-like structures around gas molecules like CO_2. Promoters enhance the stability and selectivity of these structures, making hydrates more effective for carbon capture and storage application. The carbon capture process involves interconnected processes, in particular capturing CO_2 gas from emission sources, transportation, and storage. In addition, the water separated medium for encapsulating CO_2 is considered as simple and environmentally friendly method.

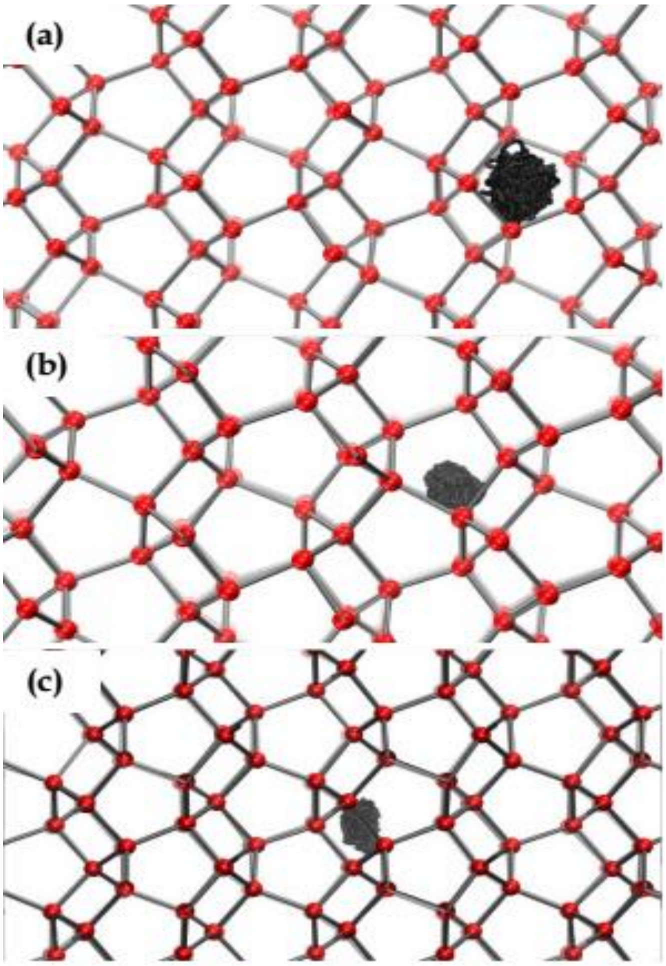

Figure 5. The CO_2 gas molecules trajectory (solid black line) inside the chiral tube along the C0 hydrate's *c* axis of (a). 200MPa, (b). 500MPa, and (c). 1000MPa system's pressure. Red spheres and gray sticks represent the hydrogen-bonded water molecules. Illustration was made using package VMD (Humphrey et al., 1996).

Conclusion

The Molecular Dynamics study on C0 hydrate was conducted by incorporating CO_2 molecules as void fillers in the ice XVII structure along the chiral tunnels parallel to the crystal's c-axis. The study utilized 324 water molecules (324 oxygen atoms and 648 hydrogen atoms), a 3×3×3 unit cell, adhering to the Bernal-Fowler rules created using the GenIce package. The CO_2 hydrate system in ice XVII with a 1:3.6 ratio was formed by adding 90 CO_2 molecules. Analyses were performed on the structure, the CO_2 gas molecule trajectories, and their diffusion coefficients within the system conditioned at a temperature of 273.15K and pressures of 200 MPa, 500 MPa, and 1000 MPa. The results indicated that the C0 hydrate pressure condition impacts the mobility of CO_2 molecules within the cage-like structure, resulting in an opposing relationship between the diffusion coefficient of CO_2 molecules and the system pressure ($5{,}03\times10^{-8}$ $cm^2\ s^{-1}$ at 200 MPa, $2{,}45\times10^{-8}$ $cm^2\ s^{-1}$ at 500 MPa, and $8{,}86\times10^{-9}$ $cm^2\ s^{-1}$ at 1000 MPa). Inter-cage hopping movement was not observed within the system evolution of 1,50 ns. The calculated diffusion coefficient of CO_2 in the C0 hydrate is larger than that of the structure 1 (S1) hydrate, indicating a relatively faster synthesis process for this hydrate. The diffusion coefficients obtained from this simulation provide insights into the dynamics of CO_2 molecules within ice XVII, aiding the development and utilization of technologies related to CO_2 interactions with the ice XVII structure.

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Author Contributions

The Conceptualization, C0 hydrate structure, post-production calculation, original draft preparation, visualization, and analysis were done by YA. A performed the molecular dynamics simulations and calculated the diffusion coefficients, while H reviewed the methods and provided supervision. All authors have read and approved the published version of the manuscript. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

The authors declare no conflict of interest.

References

Amos, D. M., Donnelly, M. E., Teeratchanan, P., Bull, C. L., Falenty, A., Kuhs, W. F., Hermann, A., & Loveday, J. S. (2017). A Chiral Gas-Hydrate Structure Common to the Carbon Dioxide-Water and Hydrogen-Water Systems. *Journal of Physical Chemistry Letters*, *8*(17), 4295–4299. https://doi.org/10.1021/acs.jpclett.7b01787

Arman, Y., & Nugroho, B. S. (2021). Molecular dynamics study of hydrogen diffusion in the C2 Hydrogen Hydrates. *Journal of Physics: Conference Series*, *1816*(1), 012084. https://doi.org/10.1088/1742-6596/1816/1/012084

Catti, M., del Rosso, L., Ulivi, L., Celli, M., Grazzi, F., & Hansen, T. C. (2019). Ne- and O_2-filled ice XVII: a neutron diffraction study. *Phys. Chem. Chem. Phys.*, *21*(27), 14671–14677. https://doi.org/10.1039/C9CP02218J

Chen, Y. A., Chu, L. K., Chu, C. K., Ohmura, R., & Chen, L. J. (2019). Synthesis of Methane Hydrate from Ice

Powder Accelerated by Doping Ethanol into Methane Gas. *Scientific Reports*, *9*(1). https://doi.org/10.1038/s41598-019-48832-8

del Rosso, L., Celli, M., Colognesi, D., Grazzi, F., & Ulivi, L. (2021). Irreversible structural changes of recovered hydrogen hydrate transforming from C0 phase to ice XVII. *Chemical Physics*, *544*, 111092. https://doi.org/10.1016/J.CHEMPHYS.2021.111092

del Rosso, L., Celli, M., Grazzi, F., Catti, M., Hansen, T. C., Fortes, A. D., & Ulivi, L. (2020). Cubic ice Ic without stacking defects obtained from ice XVII. *Nature Materials*, *19*(6), 663–668. https://doi.org/10.1038/s41563-020-0606-y

del Rosso, L., Celli, M., & Ulivi, L. (2016). New porous water ice metastable at atmospheric pressure obtained by emptying a hydrogen-filled ice. *Nature Communications*, *7*(1), 1–7. https://doi.org/10.1038/ncomms13394

del Rosso, L., Celli, M., & Ulivi, L. (2017). Ice XVII as a Novel Material for Hydrogen Storage. *Challenges*, *8*(1), 3. https://doi.org/10.3390/challe8010003

del Rosso, L., Colognesi, D., Donati, A., Rudić, S., & Celli, M. (2024). Microscopic dynamics of gas molecules confined in porous channel-like ice structure. *Journal of Chemical Physics*, *160*(15). https://doi.org/10.1063/5.0201961

del Rosso, L., Grazzi, F., Celli, M., Colognesi, D., Garcia-Sakai, V., & Ulivi, L. (2016). Refined structure of metastable ice XVII from neutron diffraction measurements. *Journal of Physical Chemistry C*, *120*(47), 26955–26959. https://doi.org/10.1021/acs.jpcc.6b10569

Dewangan, S. K., Mohan, M., Kumar, V., Sharma, A., & Ahn, B. (2022). A comprehensive review of the prospects for future hydrogen storage in materials-application and outstanding issues. *International Journal of Energy Research*, *46*(12), 16150–16177. https://doi.org/10.1002/ER.8322

Field, C. B., & Mach, K. J. (2017). Rightsizing carbon dioxide removal. *Science*, *356*(6339), 706–707. https://doi.org/10.1126/science.aam9726

Gambelli, A. M., Rossi, F., & Cotana, F. (2022). Gas Hydrates as High-Efficiency Storage System: Perspectives and Potentialities. *Energies*, *15*(22). https://doi.org/10.3390/en15228728

Harada, A., Arman, Y., & Miura, S. (2019). Molecular dynamics study on fast diffusion of hydrogen molecules in filled ice II. *Journal of Molecular Liquids*. Retrieved from https://api.semanticscholar.org/CorpusID:198346691

Hirai, H., & Kadobayashi, H. (2023). Significance of the high-pressure properties and structural evolution of gas hydrates for inferring the interior of icy bodies. *Progress in Earth and Planetary Science*, *10*(1), 3. https://doi.org/10.1186/s40645-023-00534-6

Hirai, H., Komatsu, K., Honda, M., Kawamura, T., Yamamoto, Y., & Yagi, T. (2010). Phase changes of CO_2 hydrate under high pressure and low temperature. *The Journal of Chemical Physics*, *133*(12). https://doi.org/10.1063/1.3493452

Humphrey, W., Dalke, A., & Schulten, K. (1996). VMD: visual molecular dynamics. *Journal of molecular graphics*, *14*(1), 33-38. https://doi.org/10.1016/0263-7855(96)00018-5

Ida, T., Endo, K., Matsumoto, D., Kato, N., Mizuno, M., Suzuki, Y., & Tadokoro, M. (2013). Dynamic and static behaviors of CH4 and CO2 in small and large cavities of hydrate. *Journal of Molecular Structure*, *1032*, 275–280. https://doi.org/10.1016/J.MOLSTRUC.2012.10.015

Kim, M. K., & Ahn, Y. H. (2024). Gas Hydrates for Hydrogen Storage: A Comprehensive Review and Future Prospects. *Korean Journal of Chemical Engineering*, *41*(1), 73–94. https://doi.org/10.1007/S11814-024-00025-4

Koirala, R. P., Bhusal, H. P., Khanal, S. P., & Adhikari, N. P. (2020). Effect of temperature on transport properties of cysteine in water. *AIP Advances*, *10*(2). https://doi.org/10.1063/1.5132777

Kuhs, W. F., Hansen, T. C., & Falenty, A. (2018). Filling Ices with Helium and the Formation of Helium Clathrate Hydrate. *Journal of Physical Chemistry Letters*, *9*(12), 3194–3198. https://doi.org/10.1021/ACS.JPCLETT.8B01423/SUPPL_FILE/JZ8B01423_SI_003.CIF

Liang, S., Liang, D., Wu, N., Yi, L., & Hu, G. (2016). Molecular Mechanisms of Gas Diffusion in CO_2 Hydrates. *Journal of Physical Chemistry C*, *120*(30), 16298–16304. https://doi.org/10.1021/acs.jpcc.6b03111

Liu, F. P., Li, A. R., Qing, S. L., Luo, Z. D., & Ma, Y. L. (2022). Formation kinetics, mechanism of CO_2 hydrate and its applications. *Renewable and Sustainable Energy Reviews*, *159*, 112221. https://doi.org/10.1016/J.RSER.2022.112221

Massani, B., Conway, L. J., Hermann, A., & Loveday, J. (2019). On a new nitrogen s X hydrate from ice XVII. *Journal of Chemical Physics*, *151*(10). https://doi.org/10.1063/1.5100868

Matsumoto, M., Yagasaki, T., & Tanaka, H. (2018). GenIce: Hydrogen-Disordered Ice Generator. *Journal of Computational Chemistry*, *39*(1), 61–64. https://doi.org/10.1002/jcc.25077

Michl, J., Sega, M., & Dellago, C. (2019). Phase stability of the ice XVII-based CO2 chiral hydrate from molecular dynamics simulations. *Journal of Chemical Physics*, *151*(10). https://doi.org/10.1063/1.5116540

Momma, K., & Izumi, F. (2008). VESTA: A three-dimensional visualization system for electronic and structural analysis. *Journal of Applied Crystallography*, *41*(3), 653–658. https://doi.org/10.1107/S0021889808012016

Pandey, G., Poothia, T., & Kumar, A. (2022). Hydrate based carbon capture and sequestration (HBCCS): An innovative approach towards decarbonization. *Applied Energy*, *326*, 119900. https://doi.org/10.1016/J.APENERGY.2022.119900

Pandey, J. S., Srivastava, S., Feyissa, A. H., Tariq, M., & Tumba, K. (2024). The potential role of gas hydrates: An emerging frontier in food science and engineering. *Journal of Food Engineering*, *382*. Elsevier Ltd. https://doi.org/10.1016/j.jfoodeng.2024.112210

Polat, H. M., Coelho, F. M., Vlugt, T. J. H., Mercier Franco, L. F., Tsimpanogiannis, I. N., & Moultos, O. A. (2024). Diffusivity of CO_2 in H_2O: A Review of Experimental Studies and Molecular Simulations in the Bulk and in Confinement. *Journal of Chemical & Engineering Data*. https://doi.org/10.1021/acs.jced.3c00778

Pradana, I. P., Mardiana, D., & Hakim, L. (2020). Carbon dioxide occupancies inside ice XVII structure from grand-canonical Monte Carlo simulation. *IOP Conference Series: Materials Science and Engineering*, *833*(1). https://doi.org/10.1088/1757-899X/833/1/012035

Saikia, T., Patil, S., & Sultan, A. (2023). Hydrogen Hydrate Promoters for Gas Storage—A Review. In *Energies* (Vol. 16, Issue 6). MDPI. https://doi.org/10.3390/en16062667

Strobel, T. A., Somayazulu, M., Sinogeikin, S. V., Dera, P., & Hemley, R. J. (2016). Hydrogen-Stuffed, Quartz-like Water Ice. *Journal of the American Chemical Society*, *138*(42), 13786–13789. https://doi.org/10.1021/JACS.6B06986/SUPPL_FILE/JA6B06986_SI_001.PDF

Thompson, A. P., Aktulga, H. M., Berger, R., Bolintineanu, D. S., Brown, W. M., Crozier, P. S., in 't Veld, P. J., Kohlmeyer, A., Moore, S. G., Nguyen, T. D., Shan, R., Stevens, M. J., Tranchida, J., Trott, C., & Plimpton, S. J. (2022). LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications*, *271*. https://doi.org/10.1016/j.cpc.2021.108171

Tulk, C. A., Machida, S., Klug, D. D., Lu, H., Guthrie, M., & Molaison, J. J. (2014). The structure of CO_2 hydrate between 0.7 and 1.0 GPa. *Journal of Chemical Physics*, *141*(17). https://doi.org/10.1063/1.4899265

Verstreken, M. F. K., Chanut, N., Magnin, Y., Landa, H. O. R., Denayer, J. F. M., Baron, G. V., & Ameloot, R. (2024). Mind the Gap: The Role of Mass Transfer in Shaped Nanoporous Adsorbents for Carbon Dioxide Capture. *Journal of the American Chemical Society*, *146*(34), 23633–23648. https://doi.org/10.1021/JACS.4C03086/SUPPL_FILE/JA4C03086_SI_001.PDF

Wang, X., Zhang, F., & Lipiński, W. (2020). Research progress and challenges in hydrate-based carbon dioxide capture applications. *Applied Energy*, *269*, 114928. https://doi.org/10.1016/J.APENERGY.2020.114928

Xia, Z., Li, Z., Chen, Z., Li, X., Zhang, Y., Yan, K., & Lv, Q. (2019). CO2/H2/H2O Hydrate Formation with TBAB and Nanoporous Materials. *Energy Procedia*, *158*, 5866–5871. https://doi.org/10.1016/J.EGYPRO.2019.01.539

Xu, K., Lin, Y., Li, T., Fu, Y., Zhang, Z., & Wu, J. (2022). Structural and mechanical stability of clathrate hydrates encapsulating monoatomic guest species. *Journal of Molecular Liquids*, *347*, 118391. https://doi.org/10.1016/J.MOLLIQ.2021.118391

Yang, M., Wu, M., Yang, Z., Wang, P., Chen, B., & Song, Y. (2024). Behaviors of hydrate cap formation via CO2-H2O collaborative injection:Applying to secure marine carbon storage. *Gas Science and Engineering*, *131*, 205451. https://doi.org/10.1016/J.JGSCE.2024.205451

Zhou, X., Zang, X., Long, Z., & Liang, D. (2021). Multiscale analysis of the hydrate based carbon capture from gas mixtures containing carbon dioxide. *Scientific Reports*, *11*(1), 1–9. https://doi.org/10.1038/s41598-021-88531-x