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Structure and dynamics of amorphous ice including gas molecules

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Various gaseous species such as H₂O, CO, CO₂, CH₃OH, H₂CO, and NH₃ are condensed onto dust grains in interstellar molecular clouds. The H₂O ice, which is formed by vapor deposition onto the dust grains under low temperature and pressure conditions, is amorphous ice. The amorphous ice includes various gas molecules, and the molecules undergo chemical evolutions to organic molecules through various processes [1]. Thus, the structure and properties of amorphous ice including gas molecules are important factors to understand the molecular evolution of organic molecules [2]. To investigate the effects of included gas molecules on the structure and properties of amorphous ice, the molecular dynamics (MD) calculations of amorphous ice including CO₂ and CO were performed.

We used an interatomic potential model (KAWAMURA potential model) for the MD simulations [3]. The amorphous ice

The result showed that the CO₂ molecules form a cluster when $n \geq 10$, whereas CO₂ exists as an isolated molecule i

References

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- [2]. Y. Kumagai, T. Ikeda-Fukazawa, 2017, *Chem. Phys. Lett.* 678, 153.
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Significance statement

Molecular dynamics simulations of amorphous ice including CO₂ and CO were performed. The results showed that CO₂ and CO has effects to change the density of surrounding ice matrix. From these results, we discuss the effects of gas inclusions on structure of amorphous ice.

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