

# A formation and growth model of CO<sub>2</sub> hydrate layer based on molecular dynamics

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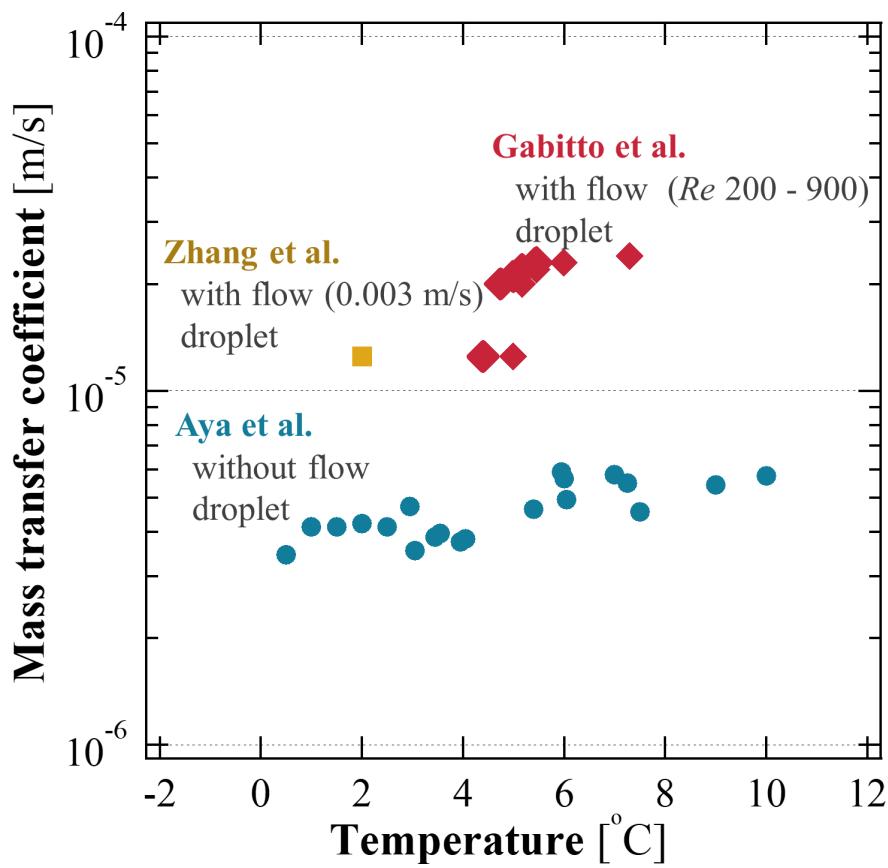
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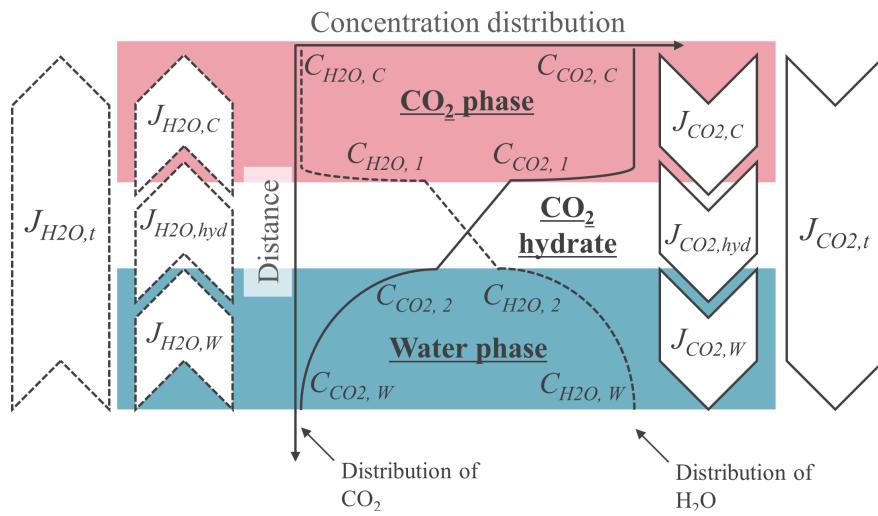
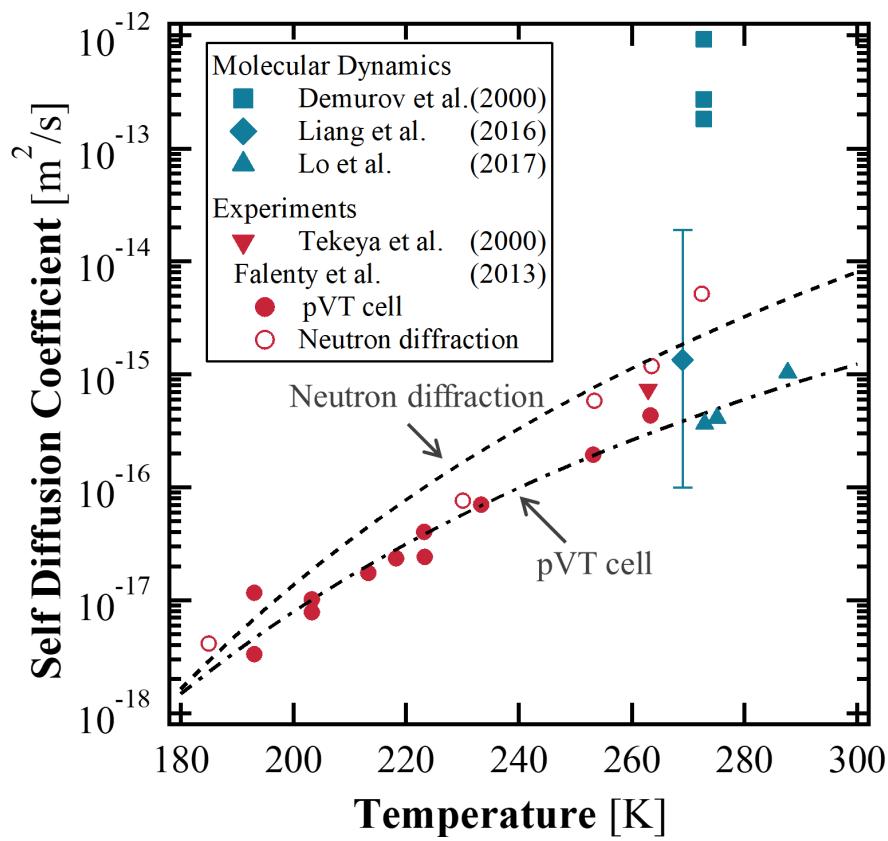
## Abstract

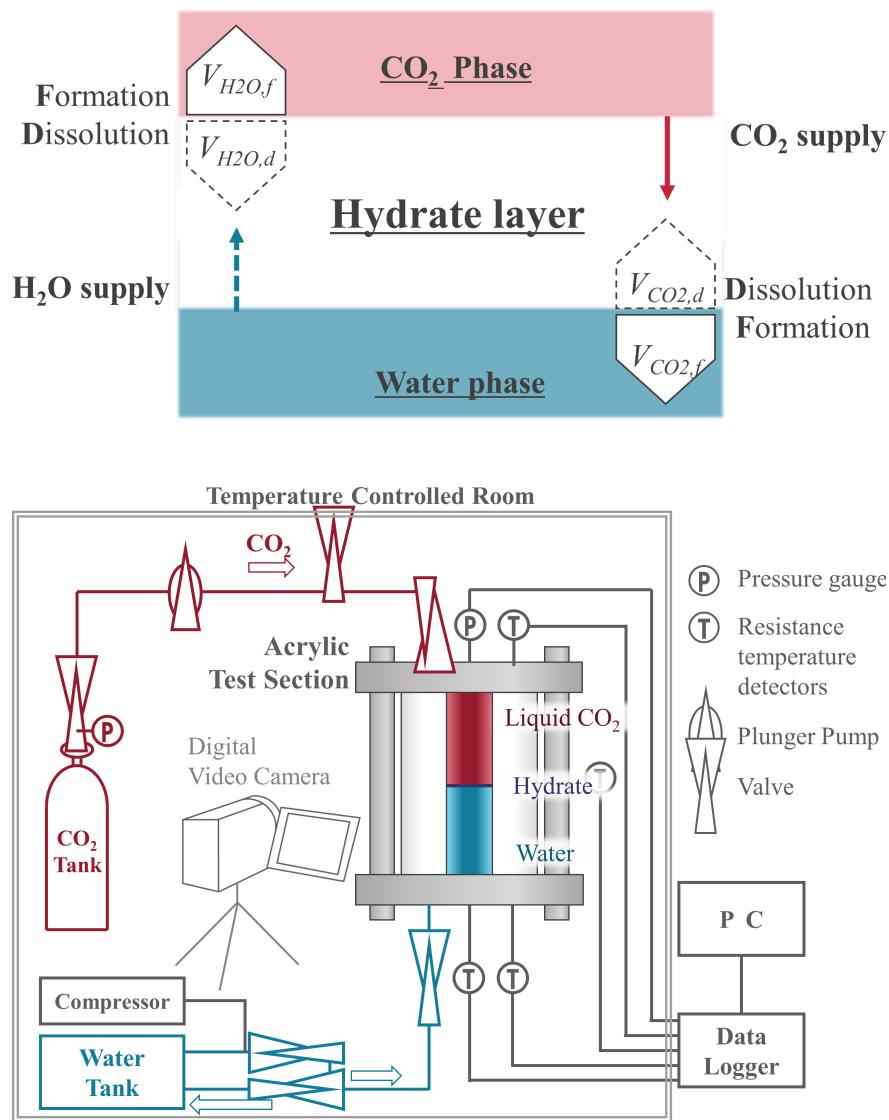
This study develops a model to predict the CO<sub>2</sub> hydrate layer thickness. As to achieve this, we need the mass transfer coefficients at the interface between water phase and CO<sub>2</sub> hydrate layer and the diffusion coefficients in CO<sub>2</sub> hydrate. Firstly, we conducted the visualization experiment of CO<sub>2</sub> hydrate layer dissolution behavior. From the experiment, we obtain the mass transfer coefficient on the CO<sub>2</sub> hydrate layer. The experimental results show good agreement with the existing empirical equation. Secondly, we conducted the molecular dynamics simulation of CO<sub>2</sub> hydrate to obtain the self-diffusion coefficients of CO<sub>2</sub> and H<sub>2</sub>O molecules. As to calculate the self-diffusion coefficients, we identified inter-cage hopping and intra-cage movement of molecules based on each molecule travel distance. Finally, the results indicate that the kinetic model we proposed reproduce the layer thickness on the order.

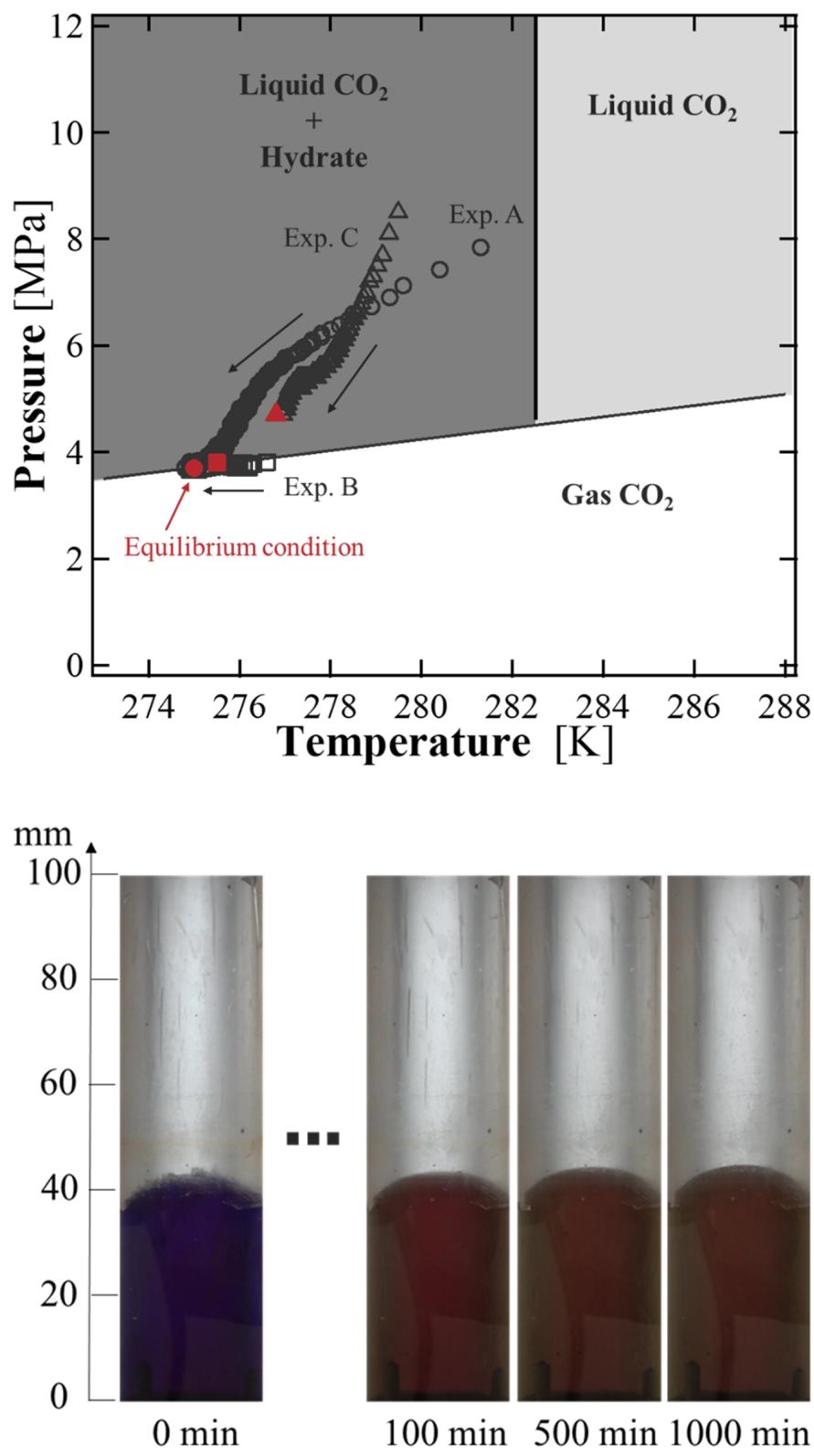
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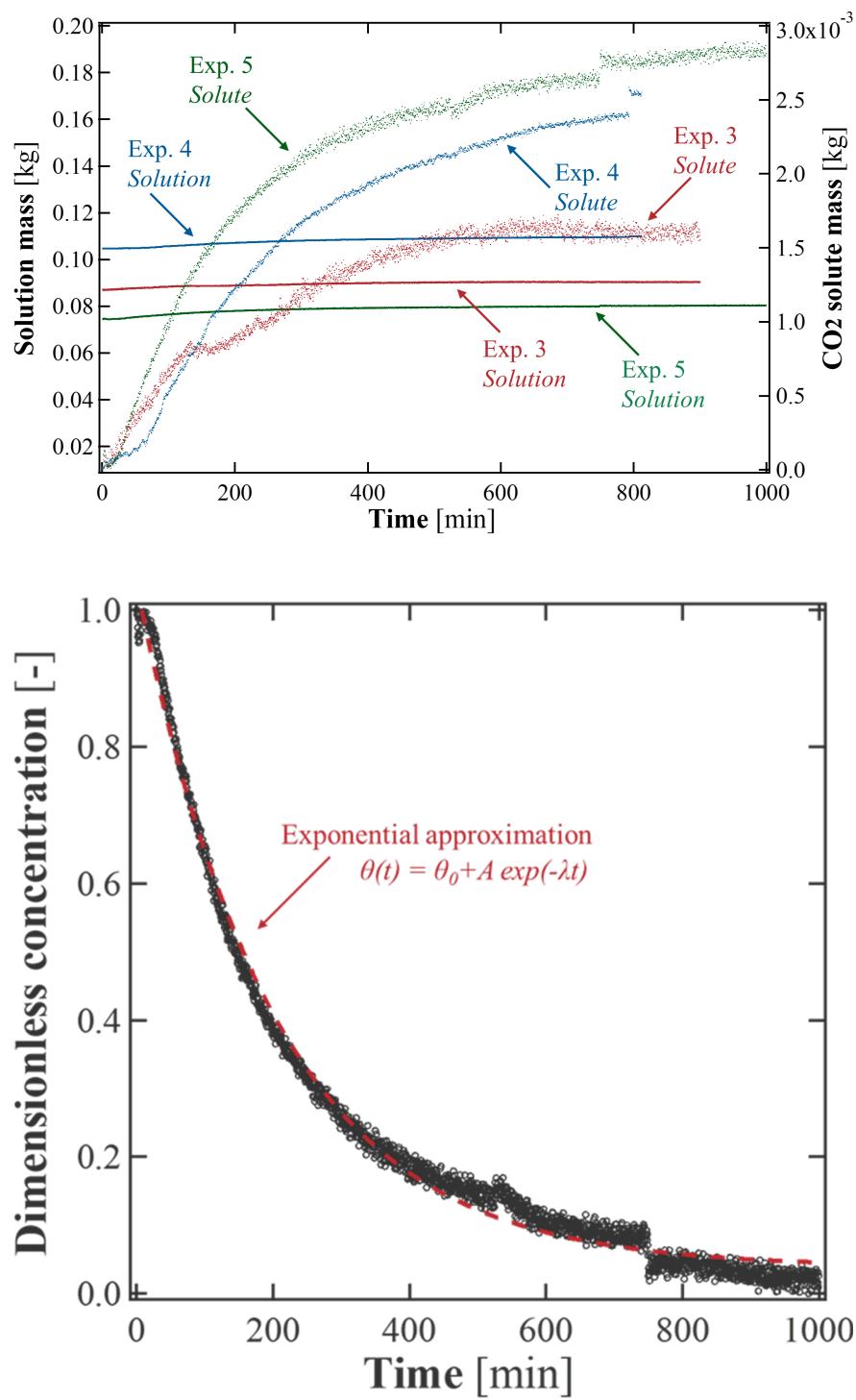
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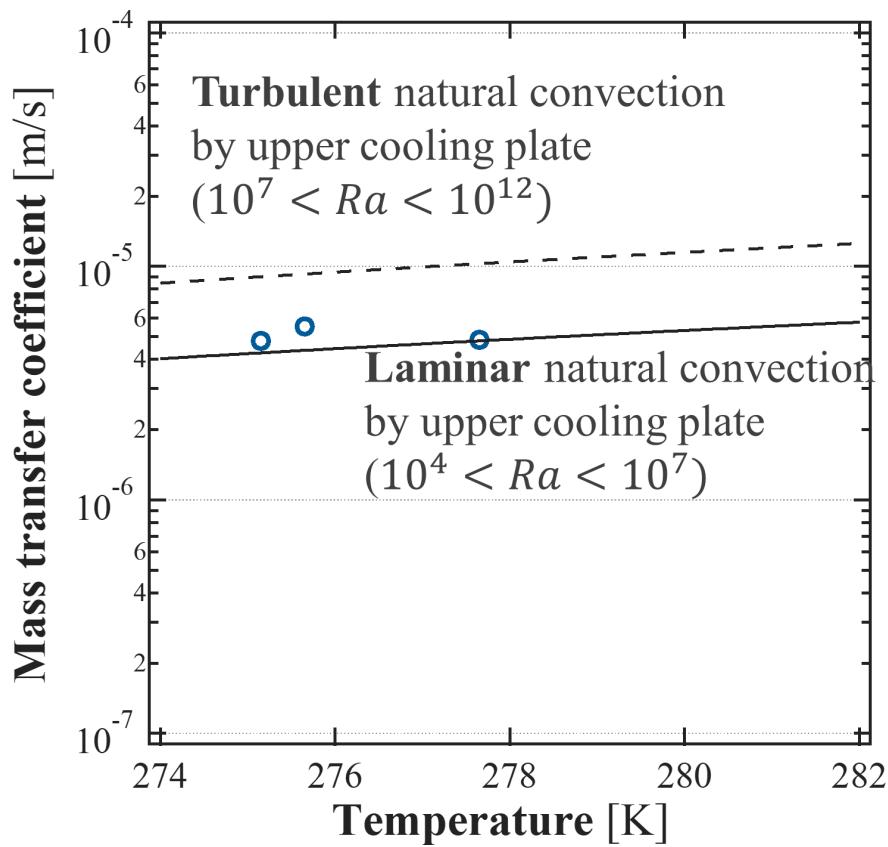


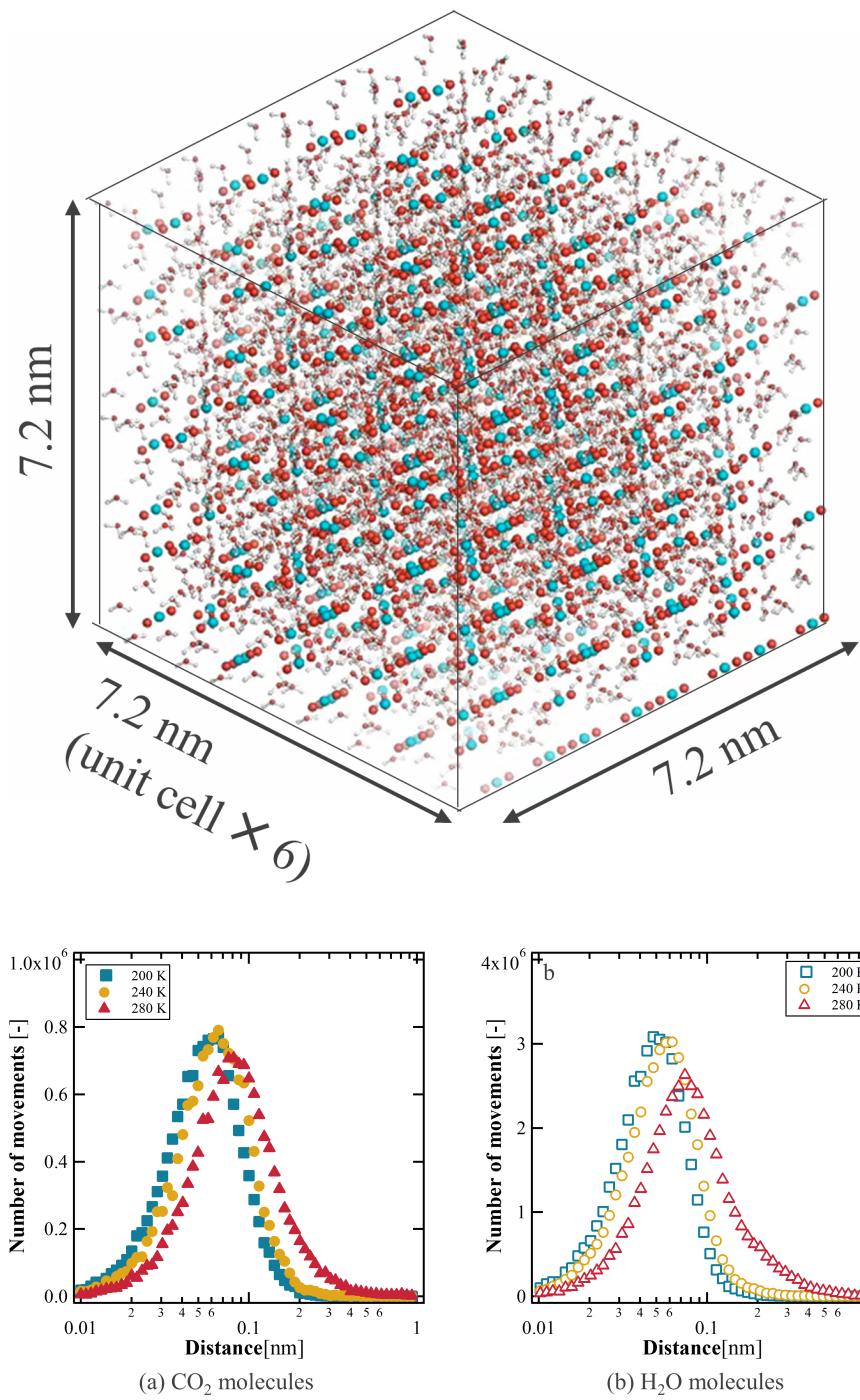


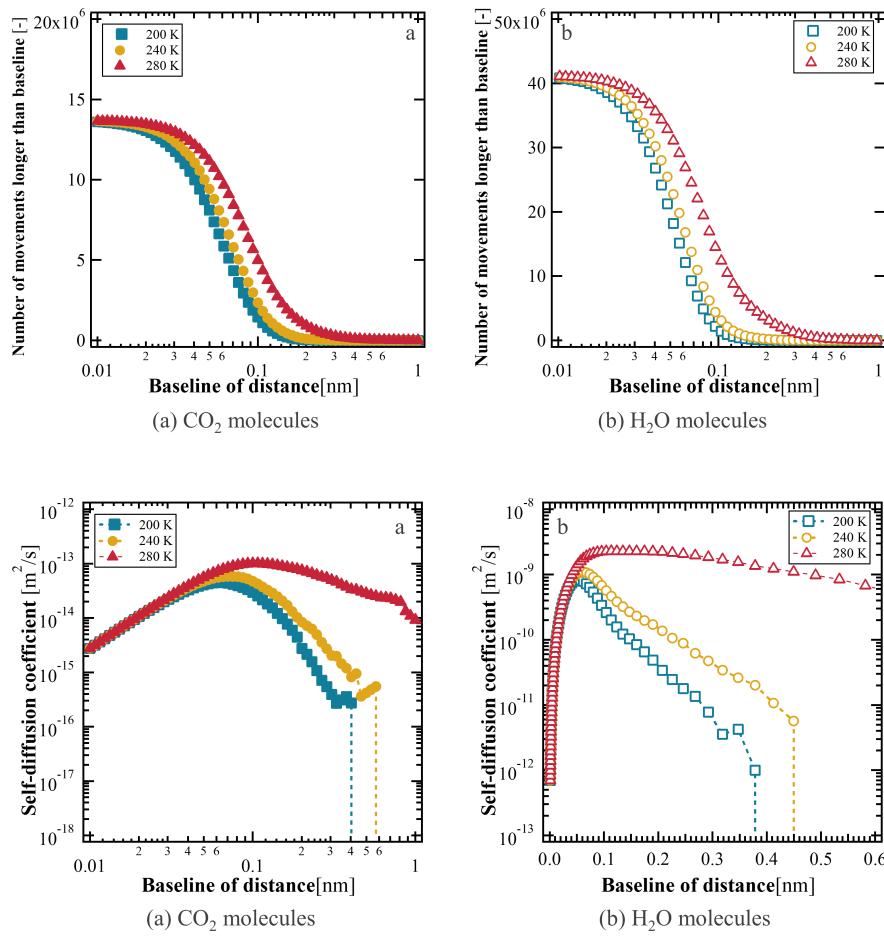


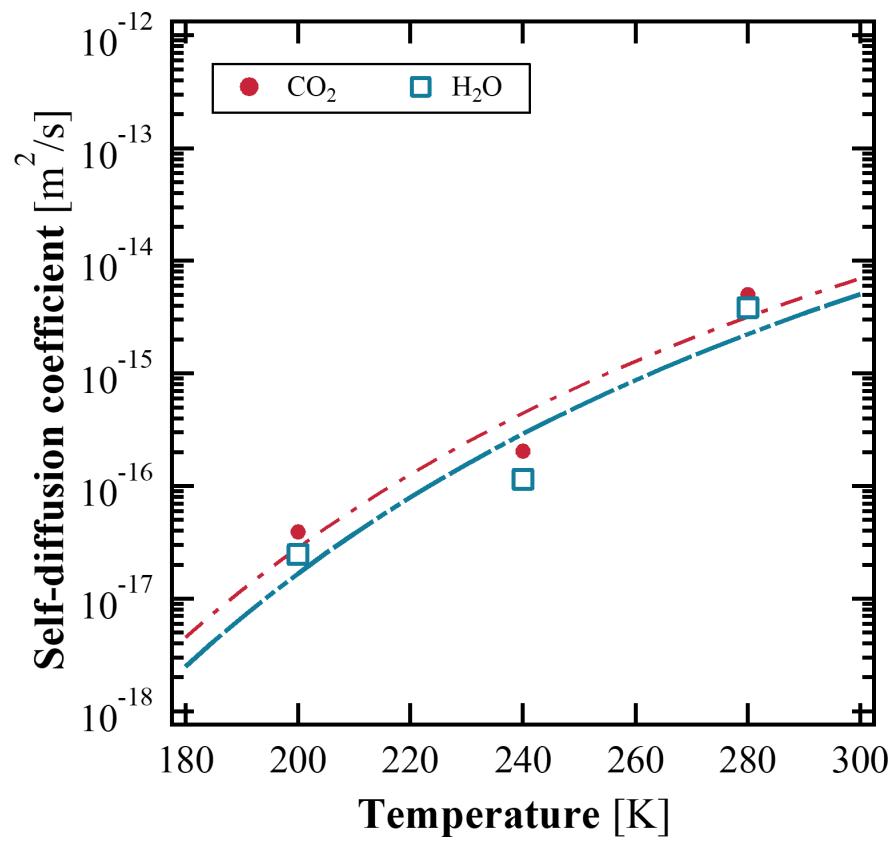


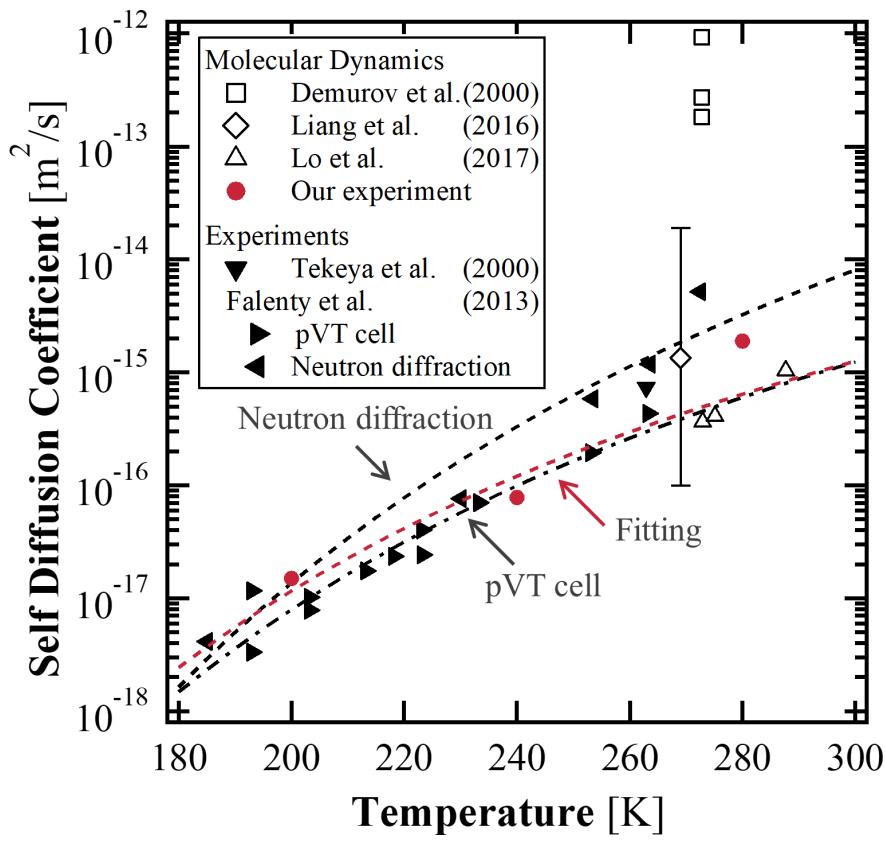


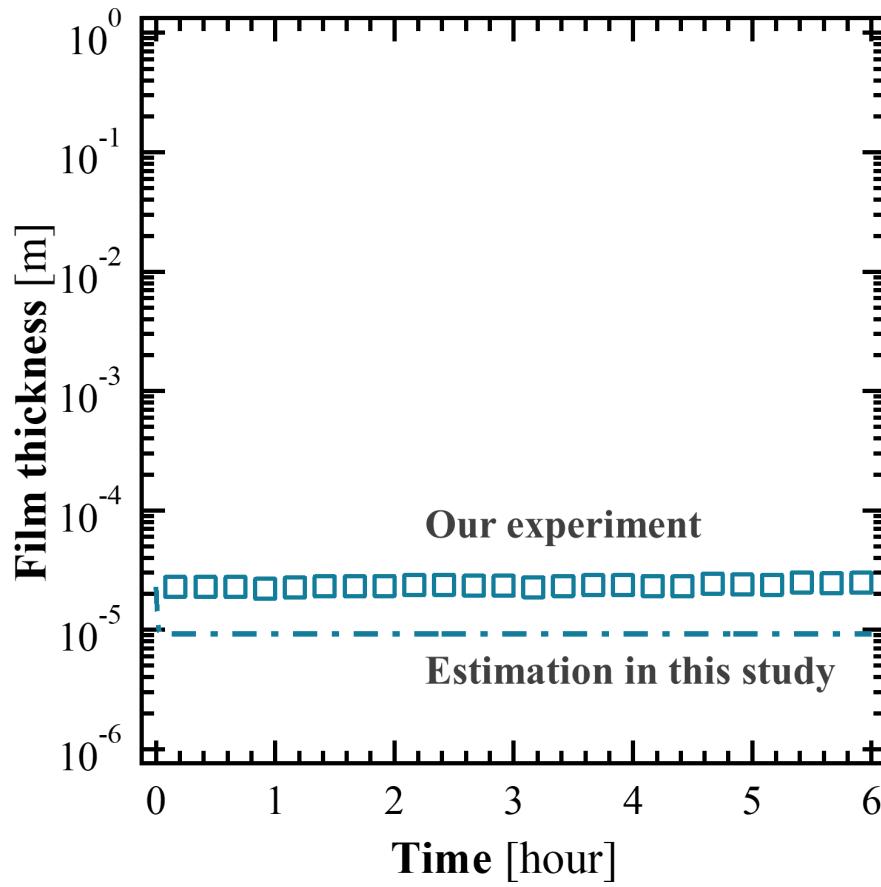












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