

PC24) Observing Oxygen Molecules Interacting with a Water Surface at Different Temperatures

Matthew Stanley Ambrosia
부산가톨릭대학교

1. 서론

Two of the most essential molecules on the earth are water and oxygen. Scientists have been studying them for centuries. In this paper a water surface and oxygen molecules were observed as they interact at the nano-scale at different temperatures.

2. 자료 및 방법

Using molecular dynamics called NAMD, a simulation was run with a water droplet with 30,968 water molecules and 501 oxygen molecules surrounding it in a fixed volume domain. Temperatures ranged from 280 K to 370 K. Interactions of the oxygen molecules and water surface were observed and analyzed.

3. 결과 및 고찰

Some oxygen molecules interacted with the water surface due to van der Waals forces, and some oxygen molecules penetrated the water surface and entered the water droplet. There was a higher possibility of the oxygen molecules to penetrate into the water surface at higher temperatures. However oxygen molecules were more likely to interact at the water surface at lower temperatures.

4. 참고문헌

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