Gwangju Institute of Science and Technology
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GIST undergraduate student participates in the bachelor's thesis research program and becomes the first-author for a paper published in an SCI-journal

☐ GIST (Gwangju Institute of Science and Technology, President Kiseon Kim) undergraduate student Seungeui Choi (senior chemistry major: advisor Professor Jun-Ho Choi) participated as the first-author of a paper published in *Physical Chemistry Chemical Physics* (PCCP), which is an SCI-level journal published by the British Royal Society of Chemistry.

- During the 2019 Fall semester, Seungeui Choi applied for a bachelor's thesis research program and participated in the GIST Department of Chemistry undergraduate research program and conducted computational chemical studies on the structure of water, which resulted in a paper published in an SCI-journal.

☐ Undergraduate Seungeui Choi applied molecular dynamics simulations* and graph theory analysis of miscibility** to three aqueous alcohol solutions of butanol at various concentrations, comparing them to other mixtures of alcohol.

> * molecular dynamics simulations: It is a theoretical way to study the behavior of atoms or molecules using Newton's equations of motion. This is a very efficient method for investigating the structure, dynamics, and thermodynamics of a molecule over time and is widely used for studying the hydrogen bond structure and motion of water in real time, which is difficult to study in experiments.

** miscibility: Miscibility is the property of two substances to mix in all proportions, forming a homogeneous solution. Two materials with similar molecular properties are generally miscible, but two materials with different properties are generally not well mixed. For example, methanol and ethanol can be mixed with water, but butanol can be partially mixed.

□ Various substances dissolved in water affect the hydrogen bonding structure and movement of water. Depending on the type, these alcohols mix well with water and sometimes tend to separate. There have been several attempts to explain this miscibility or liquid phase separation, but there has been no comparison with the quantitative explanation of how the dissolved molecules aggregate and how this affects the hydrogen bonding of water.

◦ Methanol and ethanol mix well with water regardless of concentration, but butanol at certain concentrations separates from them and from water. Interestingly, methanol, ethanol, and butanol showed little difference in the morphological structure of alcohol aggregates in a pure alcohol state without water, despite differences in their molecular properties. However, in aqueous solution, methanol and ethanol were found to be compatible with water, while butanol was not found to be compatible with water, confirming that they had different effects on the hydrogen bonding structure of water.

□ Undergraduate Seungeui Choi said, "Through this study, the collective structure of the hydrogen-bonding network of alcohol and water has been quantitatively explained, and the relationship between the morphological structure of alcohol aggregates in the aqueous solution and the mixing property of alcohol is established. Based on the results, I hope to expand to research on the effects of various molecules such as ions, osmotic substances, and proteins, as well as alcohols, on the hydrogen bond structure of water."

◦ This research was carried out with the support from the National Research Foundation of Korea and the results were published on July 8, 2020, in *Physical Chemistry Chemical Physics*, an authoritative academic journal in the field of physical chemistry.

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