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Molecular Dynamics Study of Aqueous solutions: solubility calculation and crystallization process

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Aqueous solutions are fundamental to chemistry, biology, and geology. When an aqueous solution is in high pressure and high temperature conditions, the aqueous solution becomes supercritical. It is known that the behavior of supercritical region is different from that of ambient region; however, the experimental study is very difficult. Molecular Dynamics (MD) is useful tool to observe a system in such conditions. Solubility which is one of most significant properties can be calculated with MD. Solubility calculation with MD has mainly two approaches: the free energy calculation and the direct calculation, which are thermodynamic approach and kinetic approach, respectively. The thermodynamic approach, the free energy calculation, calculates separately the values of chemical potential in solution phase and solid phase. This approach has less calculation cost and less information. The kinetic approach, the direct calculation, employs salt-solution combined system. This approach has much information which includes relaxation process. However, there is no knowledge whether two approaches produce the same solubility value or not. Thus, it is, of essential importance, to test by using two different approaches. We firstly have calculated the solubility of ambient system with the two approaches and concluded two approach had good agreement. This work will contribute to the computational chemistry field as well as solubility in supercritical region. The study at supercritical conditions is undergoing.

Keywords: sodium chloride, solubility, crystallization, molecular dynamics, supercritical solution, interface of solid