

2D Hard Sphere Free Energy Calculation through Free Volume Approach

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For the free energy calculation, statistical geometry approach has been developed and explored extensively to obtain simple yet accurate free energy value of hard-sphere system. Previous study has shown that free volume combined with Molecular Dynamics (MD) simulation can be used to estimate the free energy of 3D hard-sphere system accurately. The idea was extended to calculate the free energy of 2D hard-sphere system unlike 2D hard-disk system. Because of its close resemblance of realistic 2D material (e.g., graphene), it cannot be treated simply as the conventional disk-like 2D system, rather its 3D characteristics coming from spherical shape of atom, wrinkles, and corrugation must be taken into consideration. Thus, we employed unconfined 2D hard-sphere model. Our result shows that the free energy of 2D hard-sphere system was comparable to 2D hard-disk system only when the system height is below a dimensional transition critical point. The discrepancy can be attributed to the 3D characteristics, which could be quantified into a mathematical formulation.