عنوان مقاله:

Prediction of the phase behavior of pure polar compounds

محل انتشار:

دوازدهمین سمینار شیمی فیزیک ایران (سال: 1388)

تعداد صفحات اصل مقاله: 1

نویسندگان:

Ali Rafi Dargahi - *Department of Chemistry, College of science, Tehran University, Tehran, Iran*

Hossein Eslami - *Departemnt of Chemistry, College of science, Persian Gulf University, Boushehr, Iran*

Hassan Behnejad - *Department of Chemistry, College of science, Tehran University, Tehran, Iran*

خلاصه مقاله:

The criteria for phase equilibria requires the equivalence of temperature (thermal equilibrium), pressure (mechanical equilibrium), and chemical potential (material equilibrium) for every particle in the coexisting phases. Consequently, the chemical potential is a very important quantity, particularly for indirect methods which rely on an accurate determination of the chemicalpotential. In direct methods such as the Gibbs ensemble [1] which dose not rely on knowledge of the chemical potential, calculating the chemical potential can serve as independent verification that equilibrium has been attained. There are various methods for the calculation of chemical potential. The most common approach in this regards is the Widom test particle method [2]. The method involves inserting a ghost particle randomly into the ensemble and calculating the energy of its interaction with the particles of the ensemble. This method fails for dense fluids, big molecules, and polar compounds and needs modifications. The main disadvantage of Widom test particle is that the chemical potential is calculable just at the end of the run, instead of setting it as a target value during the period of simulation. Therefore, it is better to do simulation in the grand canonical ensemble (μVT), in which the chemical potential is constant and the number of particles change during the simulation.However, it is difficult to apply molecular dynamics in the μVT ensemble because insertion and deletion of particles can not .easily be incorporated into the equations of motion in molecular dynamics simulation

کلمات کلیدی: