Towards a DFT approach to the Mechanical Properties of Nanoporous Materials

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Résumé

Nanoporous materials exhibit unique properties due to their intricate structure, making them promising candidates for various applications. Understanding the mechanical behavior of the solid skeleton within these materials is crucial for their practical utilization. In this study, we aim at the implementation of classical density functional theory (cDFT) to explore the mechanical properties of nanoporous materials and to investigate the deformation of the solid skeleton. Classical density functional theory (cDFT) has been primarily employed for determining the structural and thermodynamic properties of inhomogeneous fluids while its application to solid phases has been explored in limited studies (1,2). Notably, prior research in this field has heavily depended on the Gaussian approximation to characterize the density distribution (3).
Two distinct approaches are employed in this study to obtain a stable solid phase within the context of classical density functional theory (cDFT). The first approach involves implementing Gaussian parametrization (equation (1)), which enables us to model a face-centered cubic (FCC) solid phase. By utilizing this approach, we were able to compute the phase diagram of a Lennard-Jones gas-liquid-FCC system, providing valuable insights into the equilibrium behavior of our system.

In the second approach, we draw inspiration from the recent work of Lutsko and Lam (3) and explore an alternative method of spontaneous crystallization without imposing a specific structure for the solid phase. Lutsko and Lam introduced a novel free energy functional that incorporates a non-local hard-sphere contribution, which exhibits improved stability when simulating a solid compared to the widely used tensorial White-Bear II (WBII) functional. Additionally, a density approximation scheme using trilinear interpolation (4) is implemented. The combination of this new free energy functional and the density approximation scheme enhances the overall, leading to spontaneous crystallization. Moreover, to investigate the deformation of nanoporous solids, we adopt the canonical ensemble instead of the conventional grand canonical one. We also test various dispersive contributions based on different potentials, including VR-Mie and WCA. As an example, Figure 1 illustrates the spontaneous localization of the density in a 2D system with VR-Mie potential obtained by using cDFT at a fixed number of particles.

By combining the cDFT approach with Gaussian parametrization and the exploration of spontaneous crystallization, this research aims to establish a solid foundation for investigating various mechanical properties associated with the solid skeleton of nanoporous materials.

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