Modelling in Materials Science by First-Principles Calculations: From Two-Dimensional Materials to Bulks

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Abstract

The first-principles density functional theory is one of the state-of-the-art methods routinely applied in electronic structure calculations. This talk provides a brief overview of the method with extensive study cases ranging from electronic properties of graphene superlattice, structural distortion and gas separation properties of porous membrane, lattice vibration of negative thermal expansion material, and defect-induced polaron formations in layered structure and bulk crystal. Together with experiment, the method has been devoted to exemplify the underlying electronic structures that relate to the properties of materials. For example, the structural deformation of porous graphene (PG) under pressure and the diffusion properties of H_2, O_2 and CO_2 through PG have been investigated. Clamped circular membrane is used to model PG subjected to a pressure difference across the membrane, the deformation of the membrane can be described by Hencky's solution. This solution provides the membrane profile and the relationship between the pressure and the blister height that can directly estimate strain in the membrane for real measurement. At a given pressure, the pressure difference across the membrane exerts strain on the surface. The relationship between strain and pressure has been obtained and used to calculate diffusion barrier of gas molecules. In the pressure range of 0-6 MPa, the diffusion rate of H_2, O_2, and CO_2 gas molecule can effectively increase by up to 7, 13, and 20 orders of magnitude, respectively. By applying sufficiently high pressure, one might able to use PG for filtering larger gas molecules such as O_2 in addition to previously proposed H_2. The results open up an opportunity to utilize PG as a controllable gas separation membrane, leading to wide range of energy and environmental applications.

Keywords: First-principles calculations, electronic structure, gas separation, graphene, polaron