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The Mechanical Property of 2D Materials and Potential Application in Gas Separation

Dong Li[1,*], Yonggang Zheng[1], Hongwu Zhang[1] and Hongfei Ye[1]

[1] International Research Center for Computational Mechanics, State Key Laboratory of Structural Analysis, Optimization and CAE Software for Industrial Equipment, Department of Engineering Mechanics, Faculty of Vehicle Engineering and Mechanics, Dalian University of Technology, Dalian, 116024, China

[*]Corresponding Author: Dong Li. Email: DongL@mail.dlut.edu.cn

ABSTRACT

The family of 2D transition-metal oxides and dichalcogenides with 1H phase (1H-MX_2) has sparked great interest from the perspective of basic physics and applied science. Interestingly, their performances could be further regulated and improved through strain engineering. Effective regulation is founded on a well-understood mechanical performance, however, the large number of 1H-MX_2 materials has not yet been revealed. Here, a general theoretical model is constructed based on the molecular mechanics, which provides an effective and rapid analytical algorithm for evaluating the mechanical properties of the entire family of 1H-MX_2. The validity of the constructed model is verified by molecular dynamics simulations upon the scale effect on the mechanical behavior of 1H-MoS_2. Notably, we report a library of the mechanical properties of 34 types of 1H-MX_2. The relevant results agree with the existing experimental and theoretical results. The relationships between the molecular structures (bond lengths and bond angles) and mechanical properties are elucidated, which offers a feasible way to predict the mechanical properties of unreported 1H-MX_2 materials. Moreover, based on the salt water-filled carbon nanotubes, a controllable 2D membrane is constructed for flow control and high-purity separation of multicomponent mixtures. The findings provide an essential theoretical basis for regulating the structures and properties of relevant materials based on atomic-scale strain engineering, which could facilitate the design and fabrication of 2D materials-based lab-on-chips, microfluidic chips, etc. The supports from NSFC (11972108, 12072061 and 12072062), LiaoNing Revitalization Talents Program (Grant No. XLYC1807193) and Fundamental Research Funds for the Central Universities are gratefully acknowledged.

KEYWORDS

2D materials; mechanical property; controllable membrane; molecular mechanics; molecular dynamics simulation

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