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Design Two-dimensional Materials with Superb Electronic and Optoelectronic Properties: The case of SiS SU-HUAI WEI, Beijing Computational Science Research Center, JI-HUI YANG, National Renewable Energy Laboratory, YUEYU ZHANG, Fudan Univeristy, WAN-JIAN YIN, Soochow University, X. G. GONG, Fudan Univeristy, BORIS I. YAKOBSON, Rice University
— Two-dimensional (2D) semiconductors have many unique electronic and optoelectronic properties that is suitable for novel device applications. Most of the current study are focused on group IV or transition metal chalcogenides. In this study, using atomic transmutation and global optimization methods, we identified two group IV-VI 2D materials, Pma2-SiS and silicene sulfide that can overcome shortcomings encountered in conventional 2D semiconducttord. Pma2-SiS is found to be both chemically, energetically, and thermally stable. Most importantly, Pma2-SiS has unique electronic and optoelectronic properties, including direct bandgaps suitable for solar cells, good mobility for nanoelectronics, good flexibility of property tuning by layer thickness and strain appliance, and good air stability as well. Therefore, Pma2-SiS is expected to be a very promising 2D material in the field of 2D electronics and optoelectronics. Silicene sulfide also shows similar properties. We believe that the designing principles and approaches used to identify these materials have great potential to accelerate future finding of new functional materials within the 2D families.

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