

Supplementary Information

The Lithium adsorption and migration in group IV-VI compounds and
GeS/graphene heterostructure: a comparative study

Kuan-Rong Hao,^a Lincan Fang,^a Qing-Bo Yan,^{*a} and Gang Su^{*b, c}

^a College of Materials Science and Opto-Electronic Technology, University of Chinese Academy of Sciences, Beijing 100049, China. E-mail: yan@ucas.ac.cn

^b School of Physical Science, University of Chinese Academy of Sciences, Beijing 100049, China. E-mail: gsu@ucas.ac.cn

^c Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China.

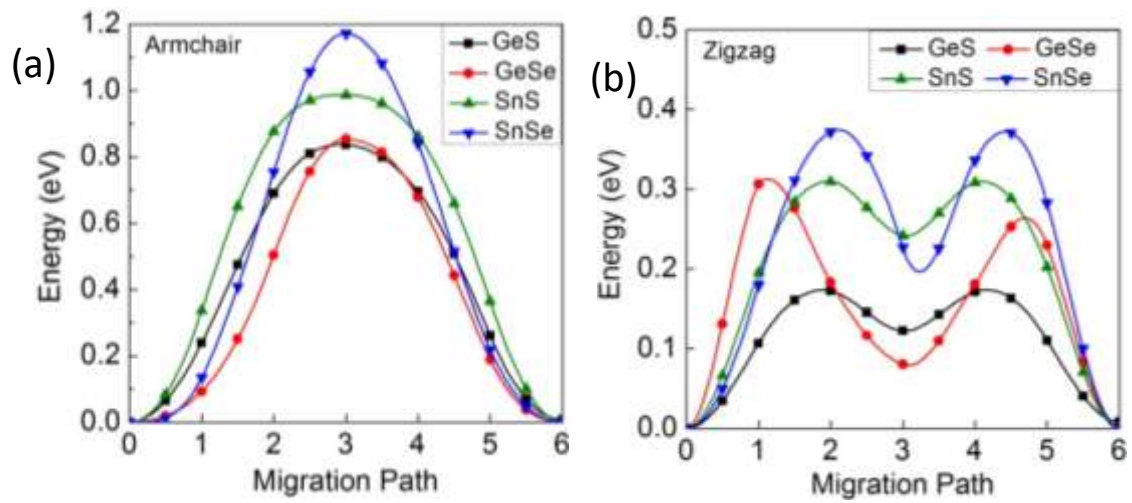


Fig. S1 (a) (b) Energy profiles of Li diffusion along armchair and zigzag directions on monolayer MX, respectively.

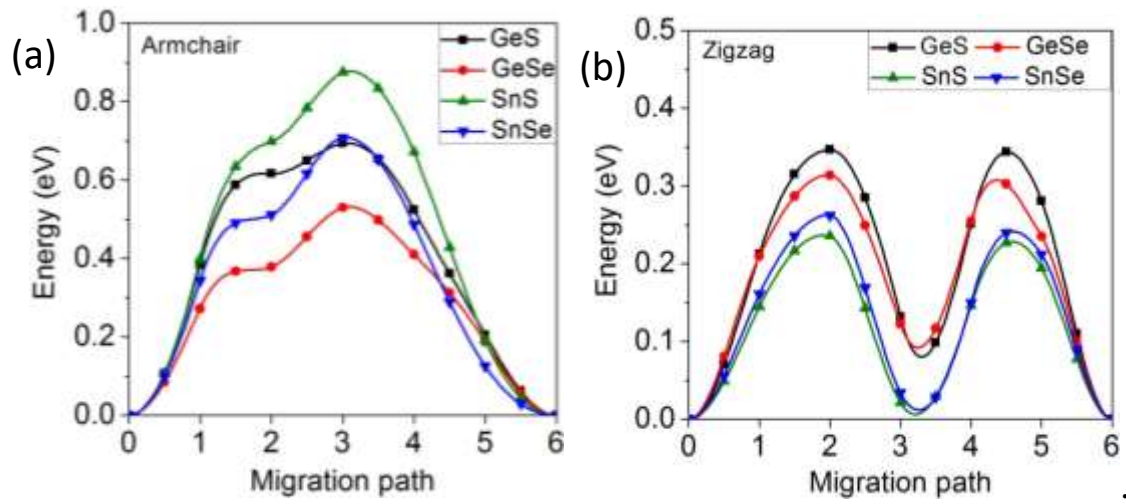


Fig. S2 (a) (b) Energy profiles of Li diffusion along armchair and zigzag directions in bulk MX, respectively.

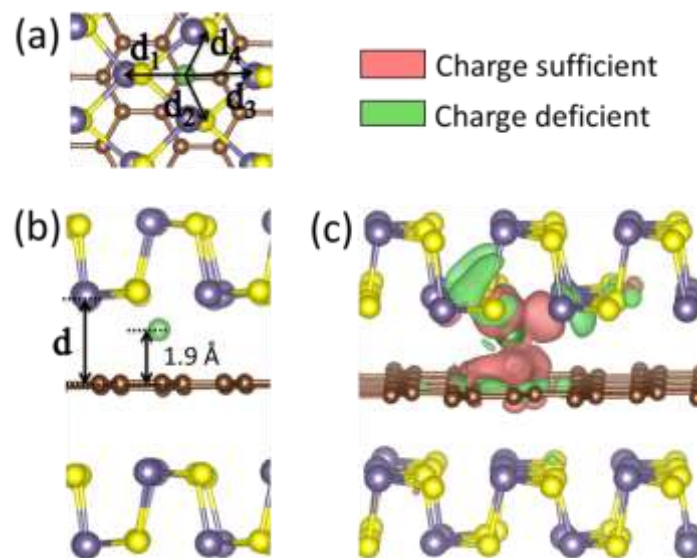


Fig. S3 (a) (b) top and side views of Li-adsorbed GeS/Graphene; (c) Differential charge density (isovalue = $0.001 \text{ e}/\text{bohr}^3$) between Li and GeS/Graphene.