Electronic Supplementary Information

New Quantum Spin Hall Insulator in Two-dimensional MoS$_2$ with Periodically Distributed Pores

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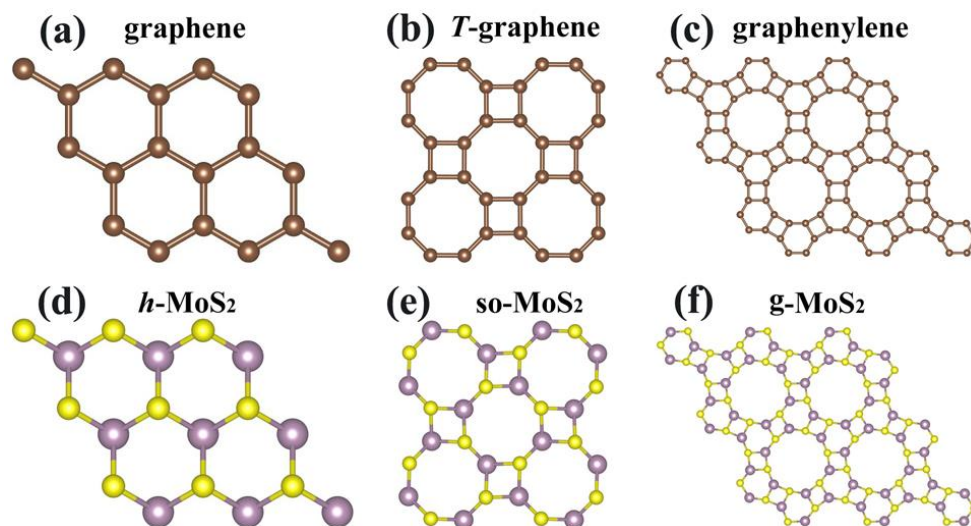[&] *Max Planck Institute for Chemical Physics of Solids, Noethnitzer Strasse 40, 01187 Dresden, Germany*

Figure S1 Top view of (a) graphene, (b) *T*-graphene,[1] (c) graphenylene,[2] (d) h-MoS$_2$, (e) so-MoS$_2$ (ref 3) and (f) g-MoS$_2$.
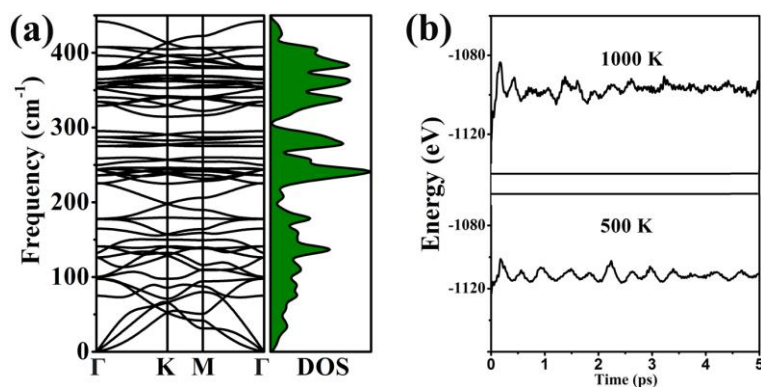

Figure S2 (a) Phonon band structure and DOS of g-MoS$_2$. (b) Energy fluctuation with respect to time in MD simulations at 500 K and 1000 K for the g-MoS$_2$. The k-point: Γ(0,0,0), K(-1/3,2/3,0), M(0,1/2,0).
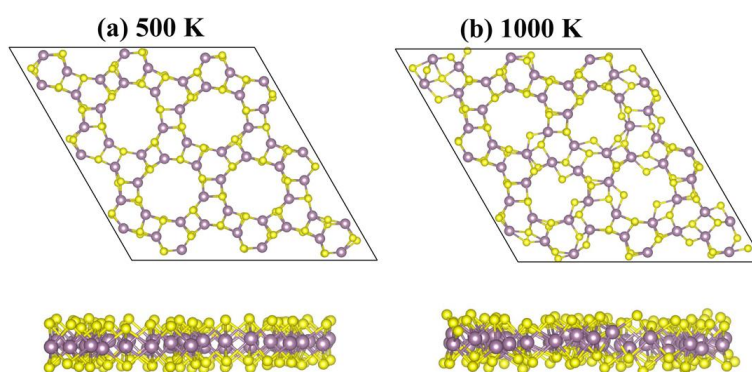

Figure S3 Top and side view of a snapshot of monolayer g-MoS$_2$ of the *ab-initio* molecular dynamics simulation at (a) 500 K and (b) 1000 K.
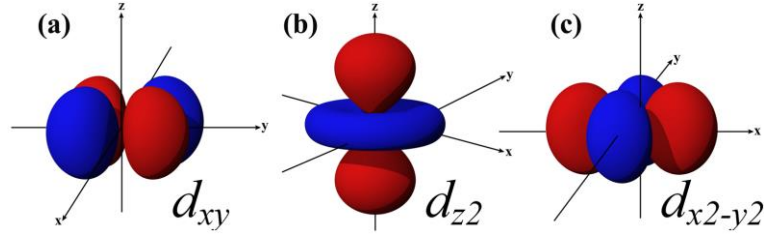
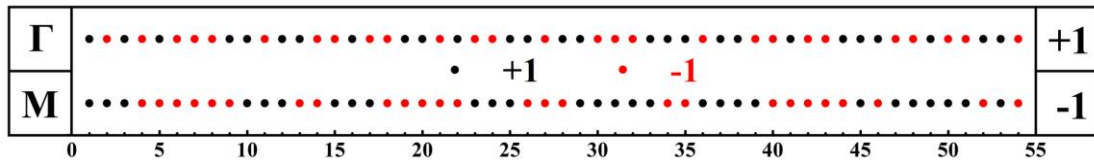Figure S4. The shapes of the three atomic d orbitals. (a) d_{xy} (b) d_{z2} and (c) d_{x2-y2}.

Figure S5. The parities of fifty-four occupied bands at Γ and three M points for g-MoS$_2$. The total number of +1 (-1) at Γ point is twenty-eight (twenty-six), while twenty-seven (twenty-seven) for M point. So it yields that the product of Γ and M points are +1 and −1, respectively.
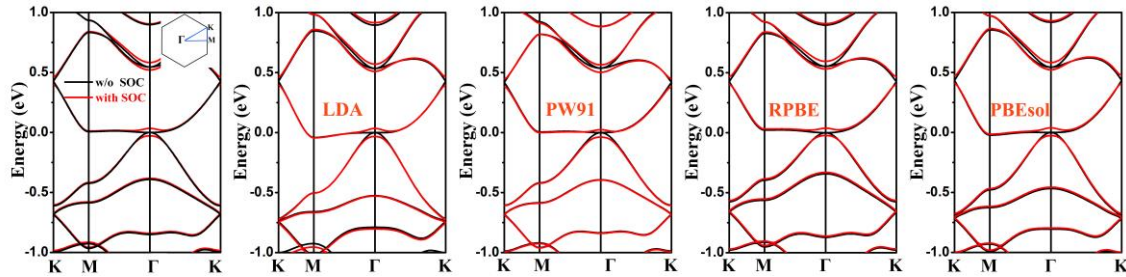

Figure S6. The calculated band structure for g-MoS$_2$ with SOC (red line) and without SOC (black line), obtained with the (a) PBE, (b) LDA, (c) PW91, (d) RPBE and (e) PBEsol functionals. The inset figure in (a) is first Brillouin zone of g-MoS$_2$ monolayer and the points of high symmetry.
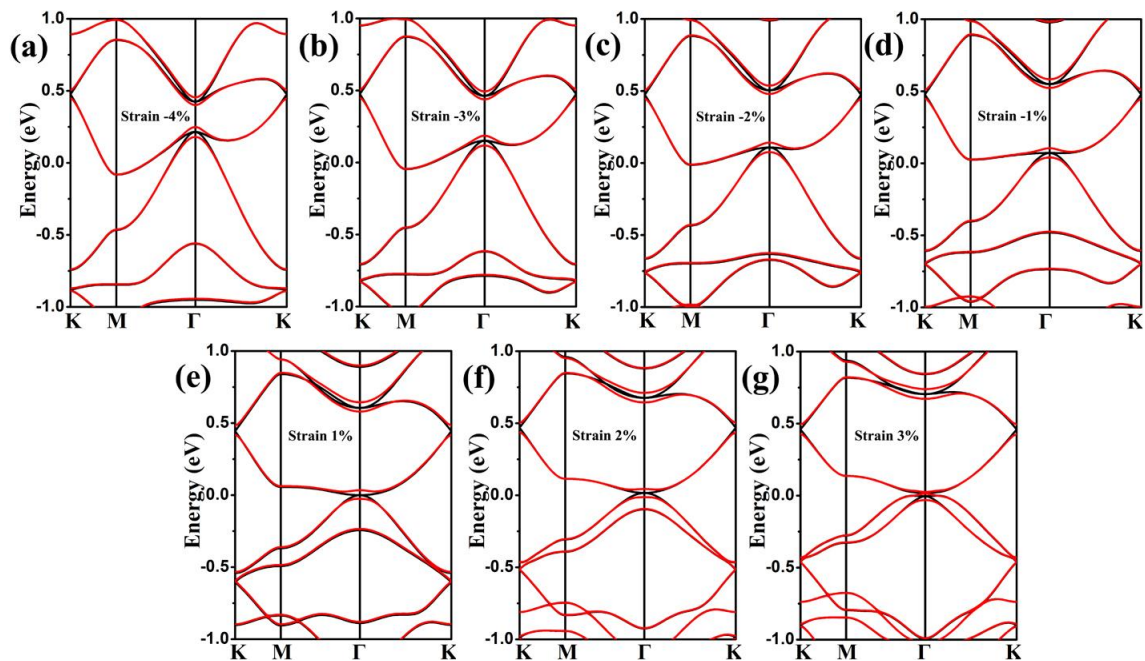
Figure S7. The calculated band structure for g-MoS$_2$ with SOC (red line) and without SOC (black line) under applied external biaxial strain in the range of −4% ~ 3%, obtained with the DFT-PBE.
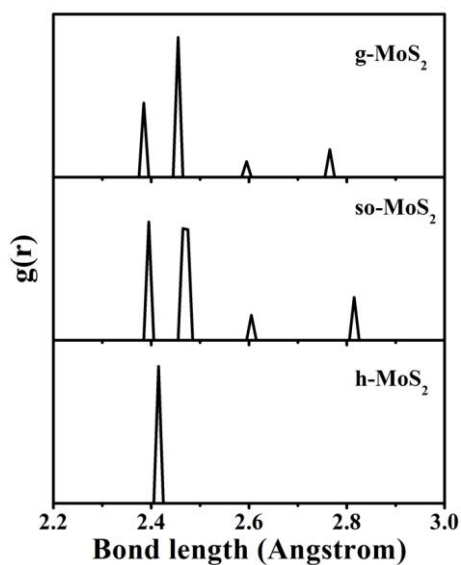

Figure S8. The Forcite analysis of bond distribution for optimized h-MoS$_2$, so-MoS$_2$ and g-MoS$_2$ monolayer. Bin size is 0.01.

References

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2. Q. Song, B. Wang, K. Deng, X. L. Feng, M. Wagner, J. D. Gale, K. Müllen and L. J. Zhi, *J. Mater. Chem.*, 2013, **1**, 38.

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