A Comprehensive DFT Study of Two-Dimensional Molybdenene and Molybdenum Carbide Phases

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S1: The crystal structures of the proposed Mo monolayers

S1.1: Atomic position of BH phase:

This file is generated by VASPKIT code

1.0

3.1292839050	0.0000000000	0.0000000000
1.5646658320	2.7101169708	0.0000000000
-0.0017818393	-0.0063344888	16.7267309597

Mo

2

Direct

0.666647017	0.666742980	0.546495974
0.333353013	0.333256990	0.453503996

S1.2: Atomic position of ZS phase:

This file is generated by VASPKIT code

1.0

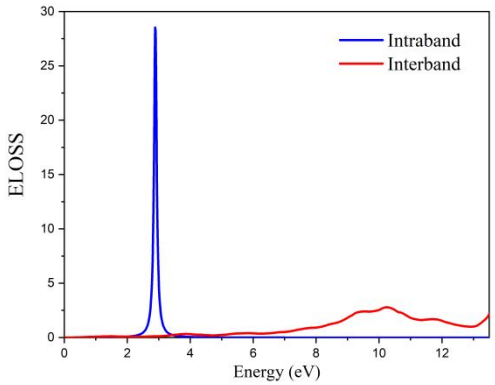
2.6312270164	0.0000000000	0.0000000000
0.0000000000	3.1025149822	0.0000000000
0.0000000000	0.0000000000	20.1910514832

Mo

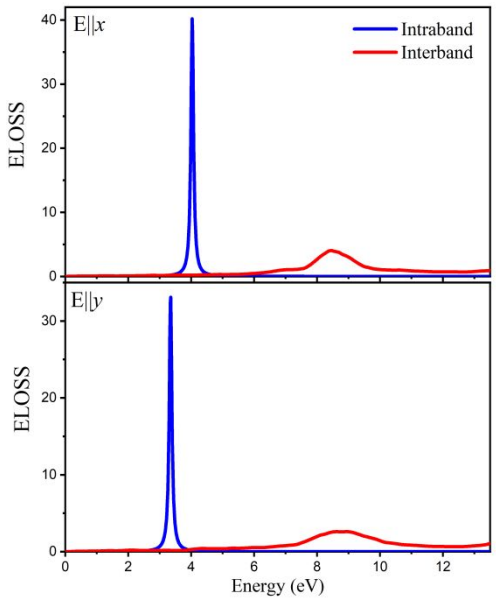
2

Direct

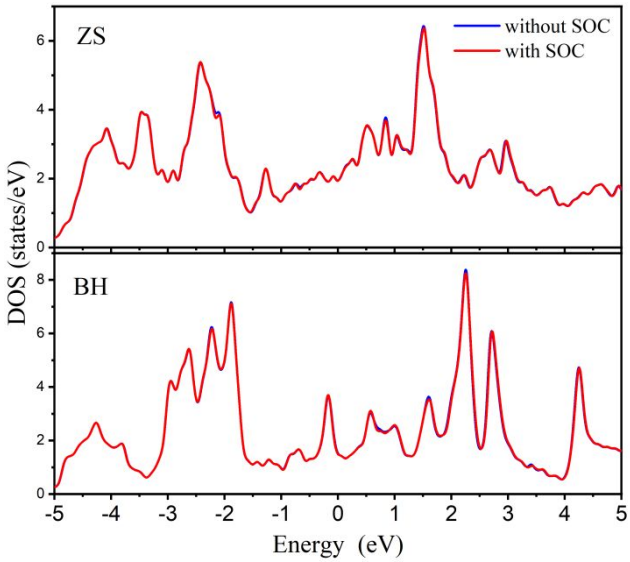
0.159856007	0.249561995	0.458617985
0.840143979	0.750437975	0.541382015



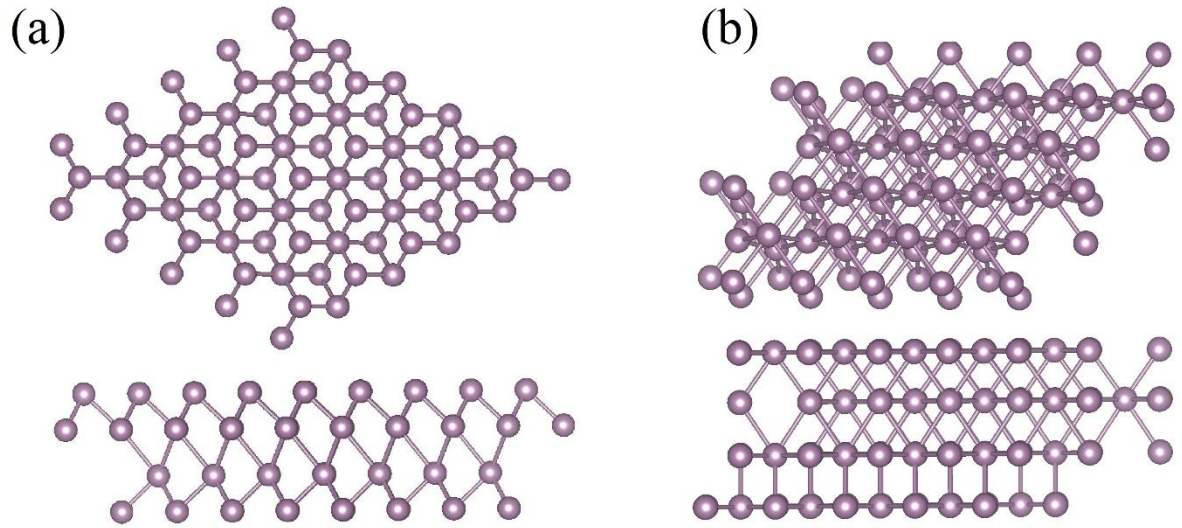
S2: Intraband and interband contributions to ELOSS function for BH phase.



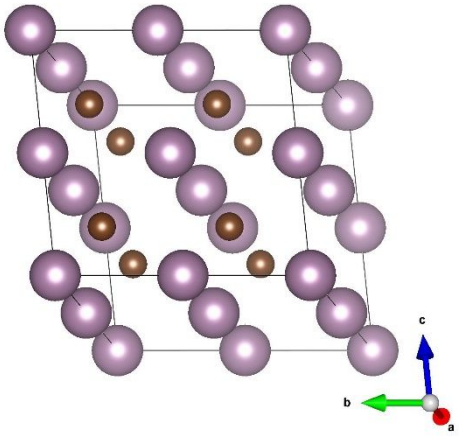
S3: Intraband and interband contributions to ELOSS function for ZS phase.



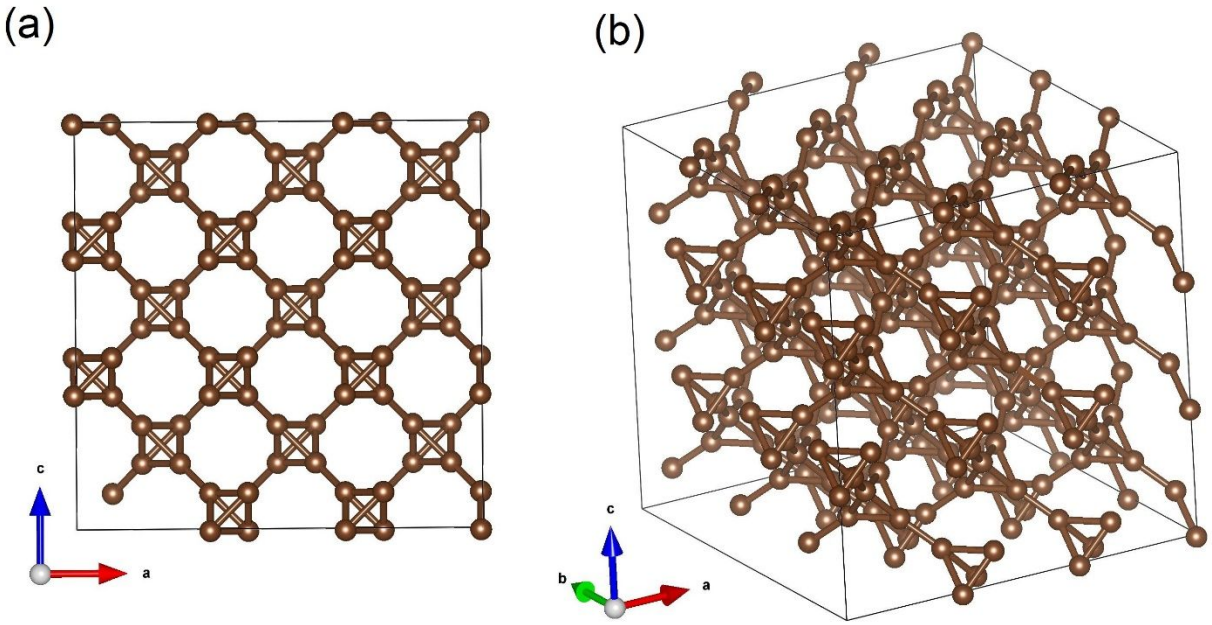
S4: Total density of states of ZS and BH molybdenene structures with and without spin-orbit coupling effect.



S5: The crystal structures of γ-DL molybdenene with the lattice parameters of a = 3.11 Å, b = 2.63 Å, $\alpha = 91.59°$,$\beta = 84.91°$, and $\gamma = 53.74°$ (a) and λ-DL molybdenene with the lattice parameters of a =b= 3.06 Å, $\alpha = \beta = 90°$, and $\gamma = 60°$ (b).



S6: Crystal structure of bulk β−MoC[1].



S7: The crystal structure of a 3×3 supercell of the T-carbon from different views[2,3].

References:

1. Liu, *et al.*, Elasticity, electronic properties and hardness of MoC investigated by first principles calculations, *Physica B: Condensed Matter* **419**, 45-50 (2013).

2. X. L. Sheng, Q. B. Yan, F. Ye, Q. R. Zheng, and G. Su, T-carbon: A novel carbon allotrope, Phys. Rev. Lett. 106(15), 155703 (2011)

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