

SUPPLEMENTARY MATERIALS

Theoretical prediction of superconductivity in two-dimensional MXenes of molybdenum carbides

Hao-Dong Liu,¹ Hong-Yan Lu,¹ Na Jiao,¹ Mengmeng Zheng,¹
Ya-Ping Li,¹ Liu Yang,¹ Bao-Tian Wang,^{2,3,4,*} and Ping Zhang^{1,5,†}

¹*School of Physics and Physical Engineering, Qufu Normal University, Qufu 273165, China*

²*Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China*

³*Spallation Neutron Source Science Center, Dongguan 523803, China*

⁴*Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, China*

⁵*Institute of Applied Physics and Computational Mathematics, Beijing 100088, China*

The structures and energy comparison of Mo_3C_2 and Mo_3C_3 systems with different configurations are shown in Figs. S1 and S2, respectively. As we can see, the most stable configurations of Mo_3C_2 and Mo_3C_3 are both 'H-1', which can be seen as the 'AA' stacking of H- Mo_2C .

In addition, we also investigate the effects of biaxial stretching on the superconducting related physical quantities of four

our studied 2D Mo_xC_y , which can be seen in Fig. S3.

As shown in Fig. S4, we explore the biaxial stretching limit of T- Mo_2C , H- Mo_2C , H- Mo_3C_2 , and H- Mo_3C_3 . Herein, we can find that when the ε is beyond the limit of biaxial stretching, the phonon dispersions of T- Mo_2C , H- Mo_3C_2 , and H- Mo_3C_3 emerge the features of CDW.

* Author to whom correspondence should be addressed. E-mail: wang-bt@ihep.ac.cn

† Author to whom correspondence should be addressed. E-mail:

zhang_ping@iapcm.ac.cn

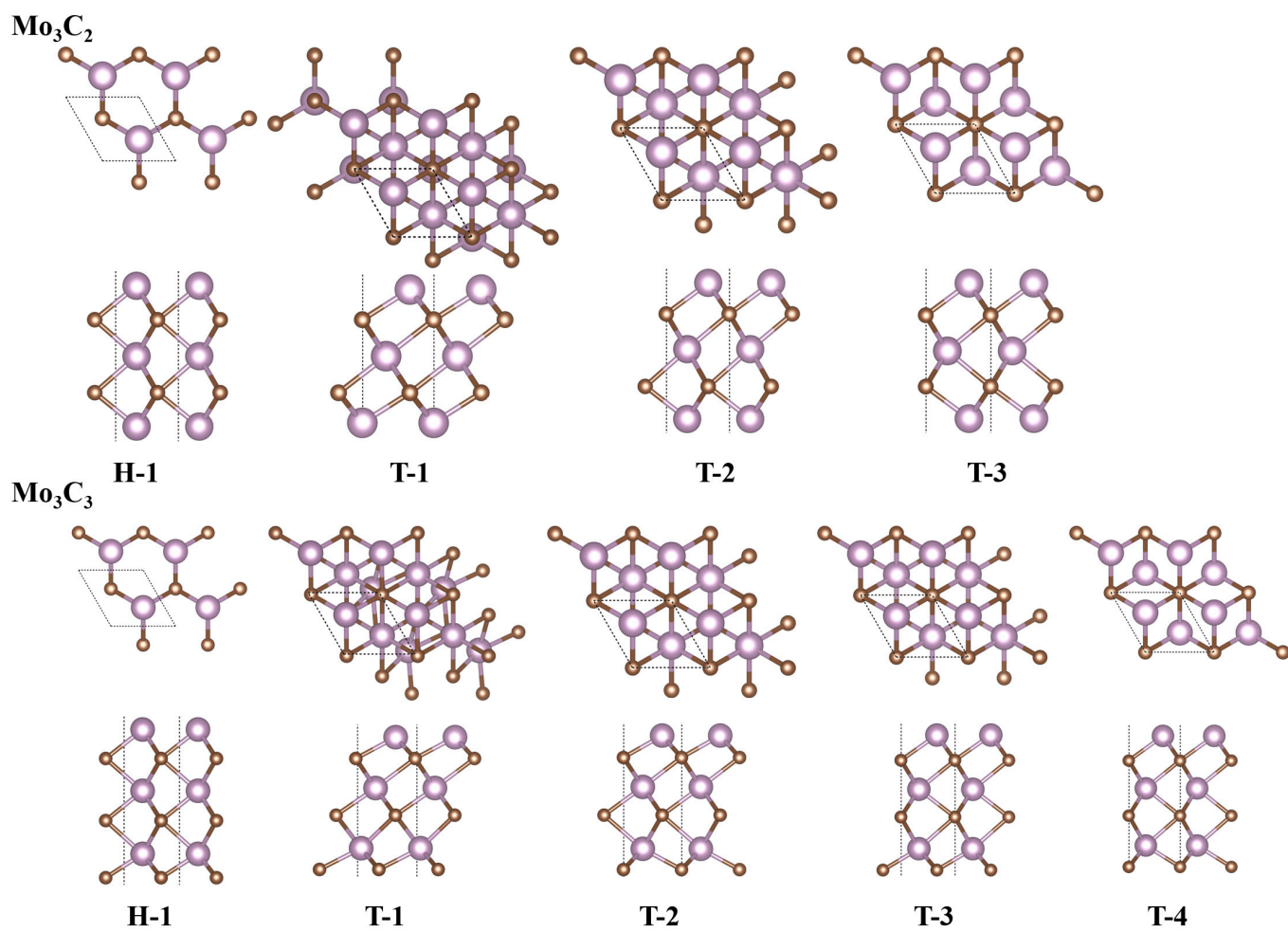


FIG. S1: The considered different structures of Mo_3C_2 and Mo_3C_3 .

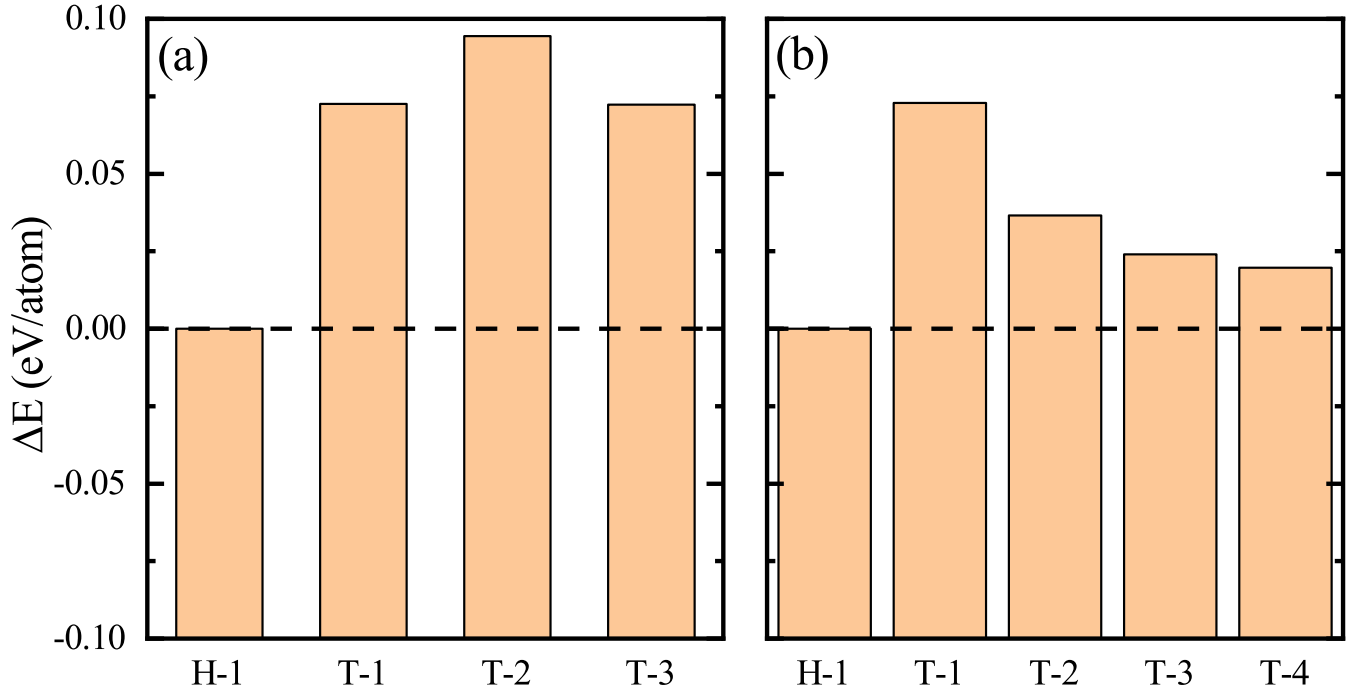


FIG. S2: Energy comparison of different configurations for (a) Mo_3C_2 and (b) Mo_3C_3 . The configurations with the lowest total energy in different systems are set to 0.0 eV/atom. The dash line are guided to the eye.

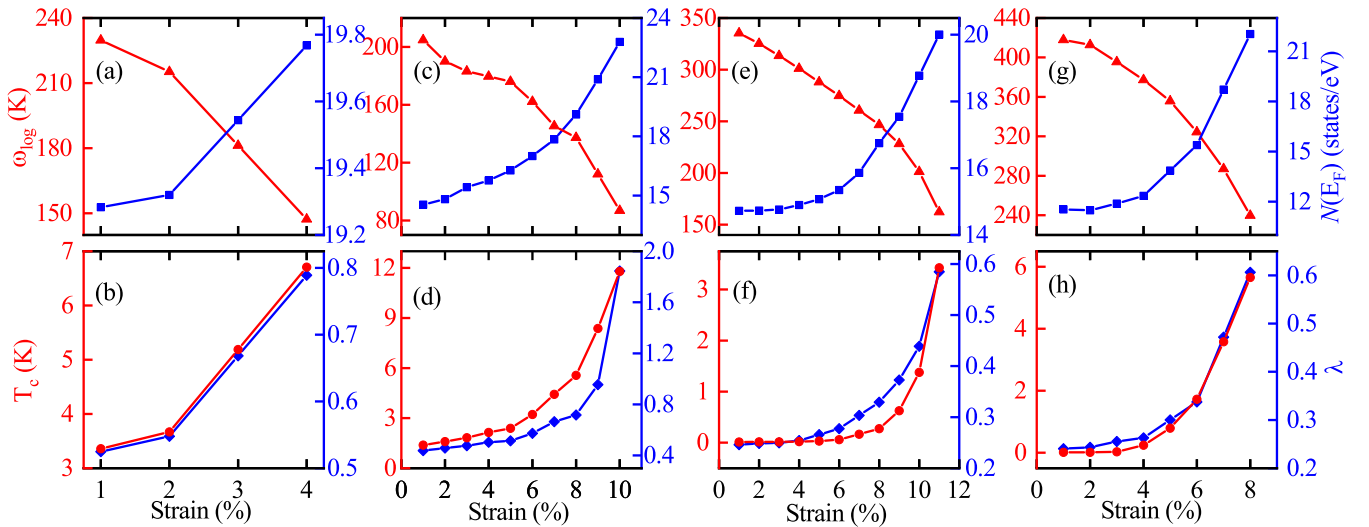


FIG. S3: The logarithmically averaged phonon frequency ω_{\log} (red), $N(E_F)$ (blue), T_c (red), and EPC constant λ (blue) under different biaxial tensile strains for (a)-(b) T- Mo_2C , (c)-(d) H- Mo_2C , (e)-(f) H- Mo_3C_2 , and (g)-(h) H- Mo_3C_3 .

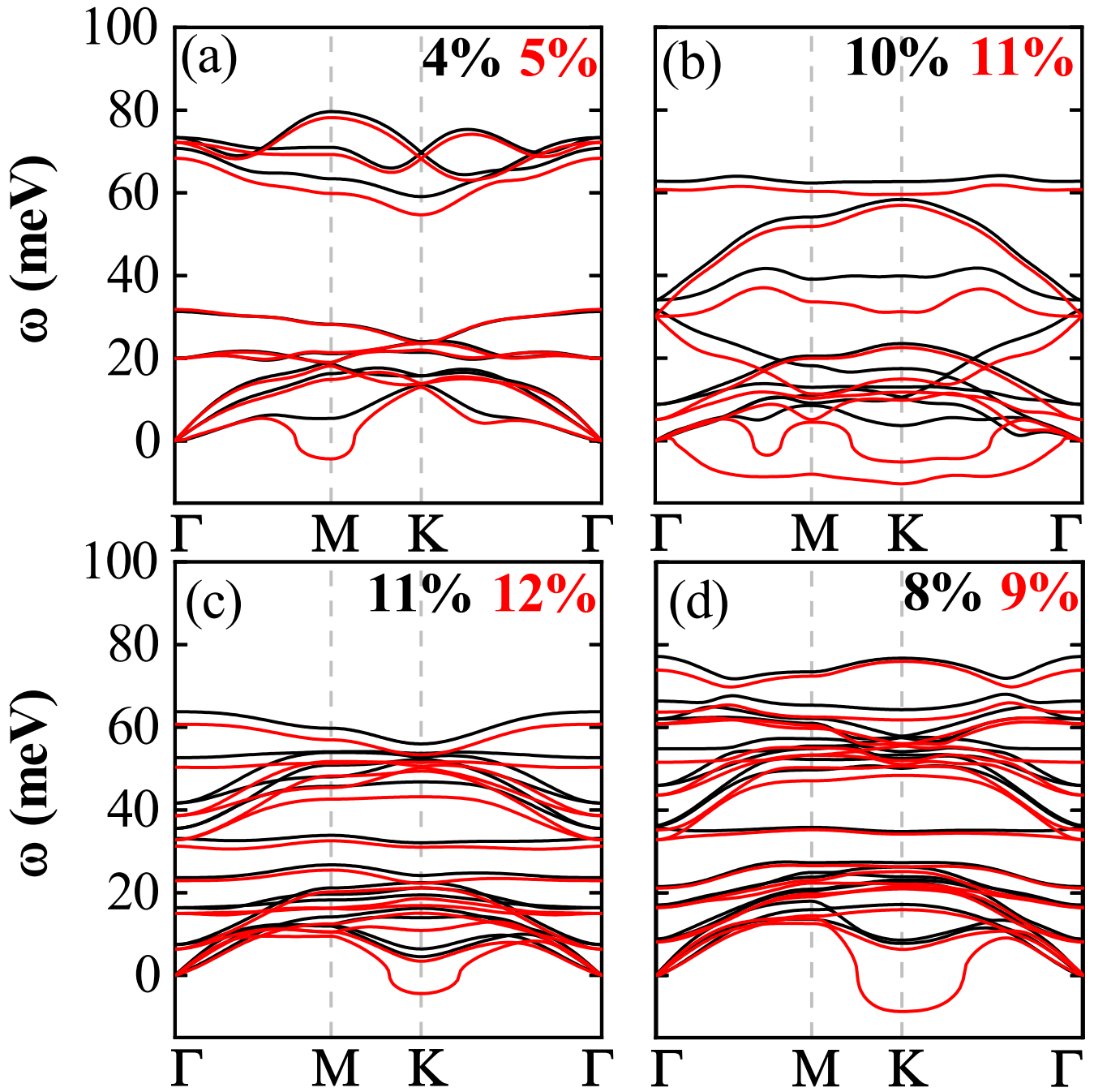


FIG. S4: The phonon spectra of (a) T-Mo₂C, (b) H-Mo₂C, (c) H-Mo₃C₂, and (d) H-Mo₃C₃ beyond the limit of biaxial stretching.