

Supporting Information

Engineering Electronic Structures and Optical Properties of MoSi₂N₄ Monolayer via Modulating Surface Hydrogen Chemisorption

Yumei Zhang ^a, Shunhong Dong ^a, Pachaiyappan Murugan ^a, Ting Zhu ^{a,b}, Chen Qing ^a, Zhiyong Liu ^{a,b,*}, Weibin Zhang ^{a,b,*}, Hong-En Wang ^{a,b,*}

^a Yunnan Key Laboratory of Optoelectronic Information Technology, College of Physics and Electronic Information, Yunnan Normal University, Kunming 650500, China.

^b Key Laboratory of Advanced Technique & Preparation for Renewable Energy Materials, Ministry of Education, Yunnan Normal University, China.

Correspondence should be addressed to:

Email(s): liuzhiyong@ynnu.edu.cn (Z. Liu), 220001@ynnu.edu.cn (W. Zhang), hongen.wang@outlook.com (H.-E. Wang)

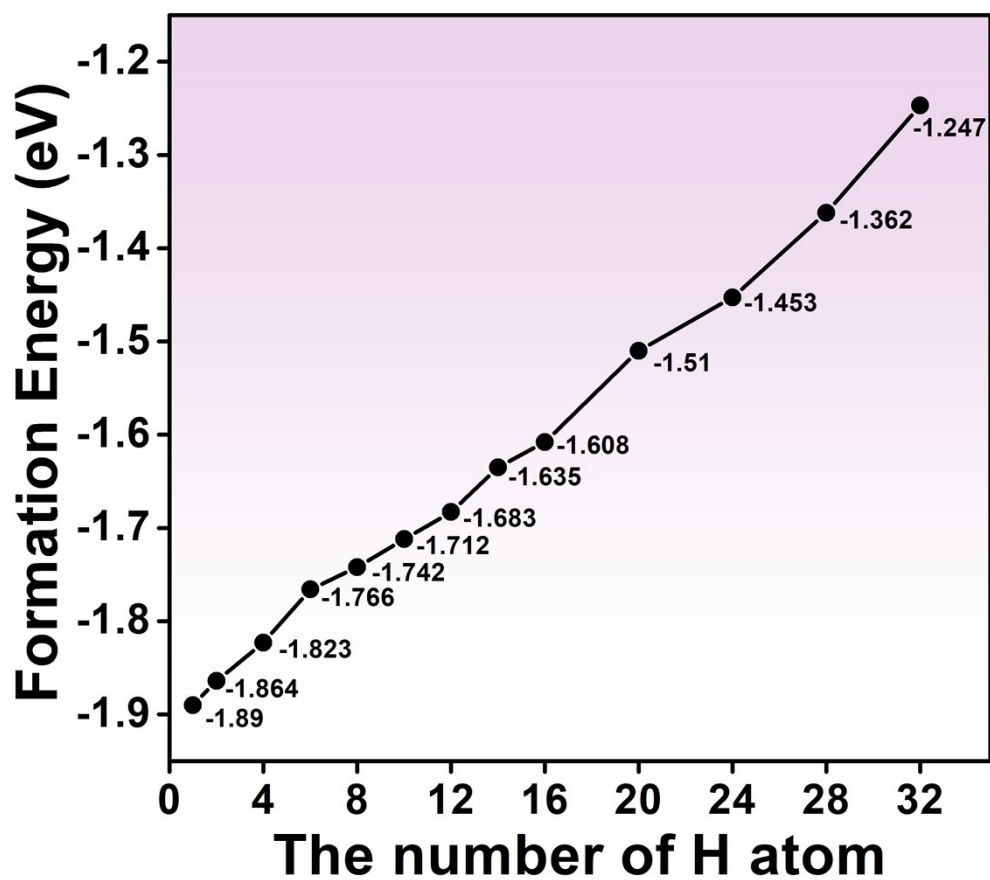


Fig. S1. The formation energies of $n\text{H-MoSi}_2\text{N}_4$ as a function of n . Herein n represents the number of H atoms chemisorbed on MoSi_2N_4 surface.