Supporting Information

Mechanical, electronic and catalytic properties of 2H-1T' MoS_2 heterointerfaces

Xiangru Huang[a,b], Yuan Chang[a], Shi Qiu[a], Hongsheng Liu[*a], Vitali Shymanski[b] and Junfeng Gao[*a,b]

[a] *Key Laboratory of Materials Modification by Laser, Ion and Electron Beams* (*Dalian University of Technology*), *Ministry of Education, Dalian 116024, China.* email: gaojf@dlut.edu.cn; liuhongsheng@dlut.edu.cn

[b] *Dalian University of Technology and Belarusian State University Joint Institute- Innovation Center.*

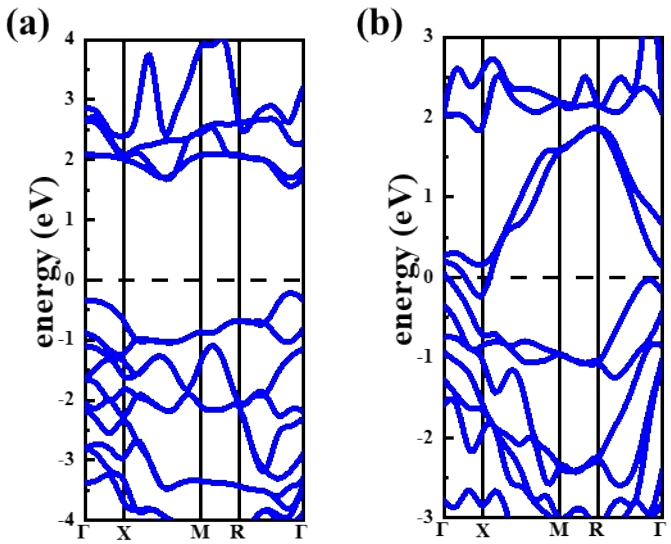

Figure S1. (a) Electronic band structure of 2H-MoS_2. (b) Electronic band structure of 1T'-MoS_2.

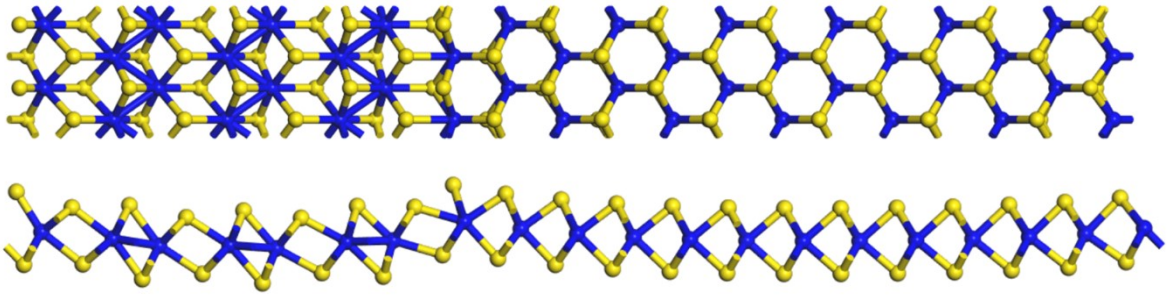

Figure S2. Top and side views of the S-LU-sint heterostructure by doubling the domain size of both 2H and 1T' phases in the manuscript.

Table S1. Hydrogen chemisorption energy (ΔE_H), zero-point energy ($\Delta E_{zero\ point}$), entropy and Gibbs free energy for hydrogen adsorbed on different sites of S-LU-sint

Site	ΔE_H**(eV)**	$\Delta E_{zero\ point}$**(eV)**	$T\Delta S$**(eV)**	ΔG**(eV)**
Interface	-0.271	0.249	0.0057	-0.028
Far from interface in 1T' phase	-0.042	0.252	0.006	0.204
Near interface in 1T' phase	0.037	0.249	0.007	0.279
Near interface in 2H phase	1.395	0.219	0.005	1.610
Far from interface in 2H phase	1.378	0.219	0.006	1.590