

Supporting Information

First-Principle Investigations of Vanadium Disulfide for
Lithium and Sodium Ion Battery Applications

Wenhui Wang¹, Zhongti Sun¹, Wenshuai Zhang², Quanping Fan³, Qi Sun¹, Xudong
Cui^{4*}, Bin Xiang^{1*}

¹Department of Materials Science & Engineering, CAS Key Lab of Materials for Energy Conversion, Synergetic Innovation Center of Quantum Information Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China.

²Network Information Center, Supercomputing Center, University of Science and Technology of China, Hefei 230026, China.

³Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China.

⁴Science and Technology on Plasma Physics Laboratory, Research Center of Laser Fusion, CAEP, Sichuan, 621900, China.

*Corresponding author: binxiang@ustc.edu.cn; xudcui@163.com

Figures

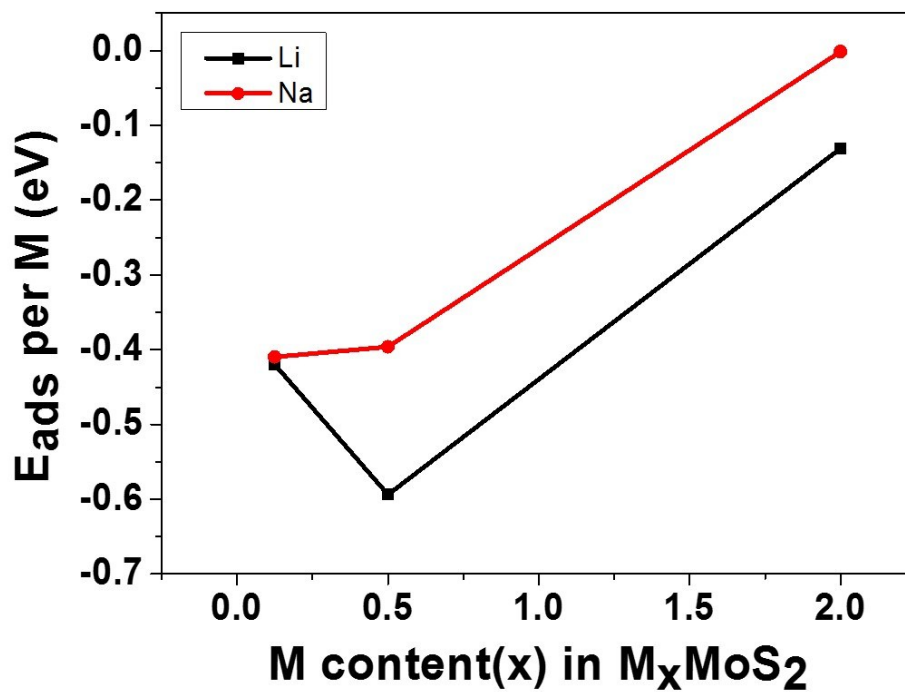


Figure S1. The adsorption energy of bulk MoS_2 for lithium and sodium ions batteries

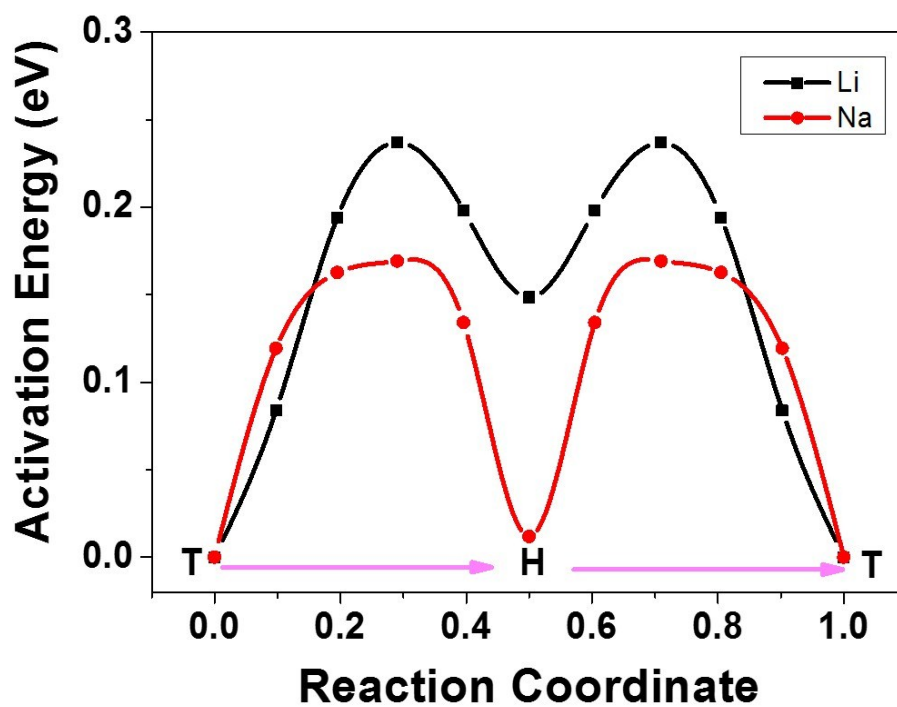


Figure S2. Activation energy barrier for the Li⁺ and Na⁺ diffusions in the monolayer MoS₂

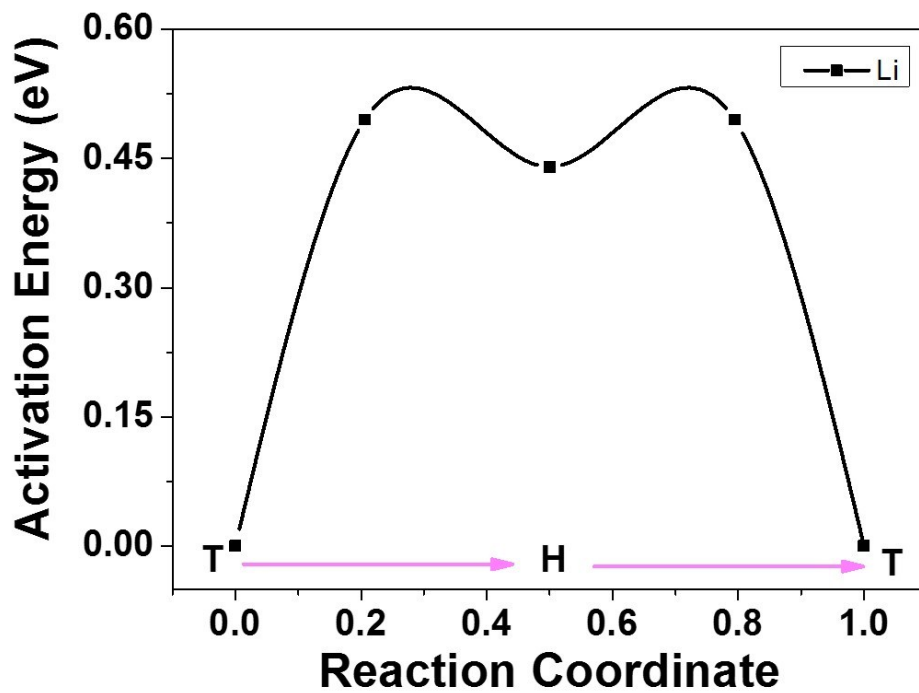


Figure S3. Activation energy barrier for the Li^+ diffusion in the bulk

MoS_2

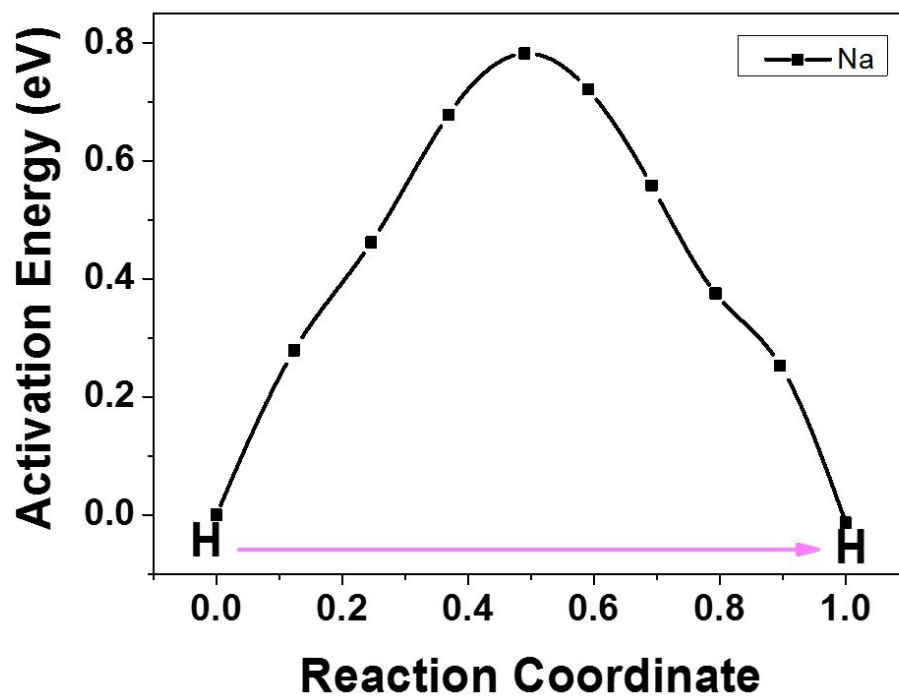


Figure S4. Activation energy barrier for the Na⁺ diffusion in the bulk

MoS₂