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Electronic Supplementary Information (ESI) for

Hydrogen-induced Structural Stability and Promising Electronic Properties of Molybdenum and Tungsten Dinitride Nanosheets: A First-principles Study

Yanli Wang*[a] and Yi Ding*[b]

a. Department of Physics, Center for Optoelectronics Materials and Devices, Zhejiang Sci-Tech University, Xiasha College Park, Hangzhou, Zhejiang 310018, People's Republic of China. Email: wangyanli-04@tsinghua.org.cn

b. Department of Physics, Hangzhou Normal University, Hangzhou, Zhejiang 310036, People's Republic of China. E-mail: dingyi2001@tsinghua.org.cn

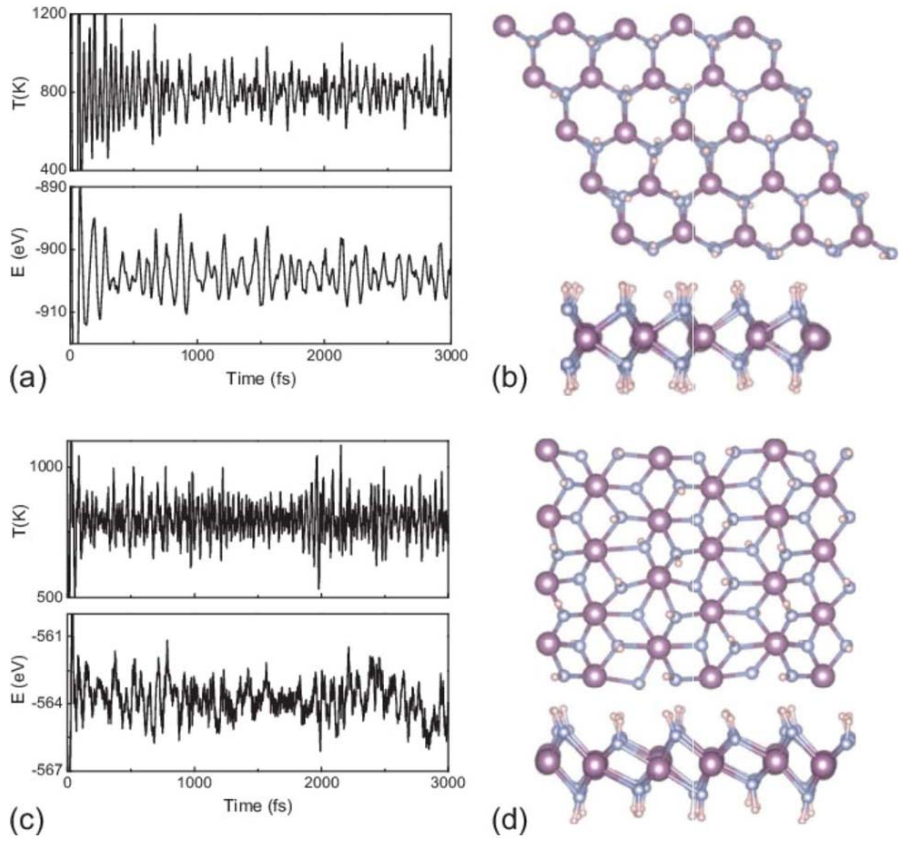

Figure S1. The fluctuations of temperature and free energy, as well as the final structures after the AIMD simulations for [(a), (b)] $H-MoN_2H_2$ and [(c), (d)] $T_d-MoN_2H_2$ sheets.

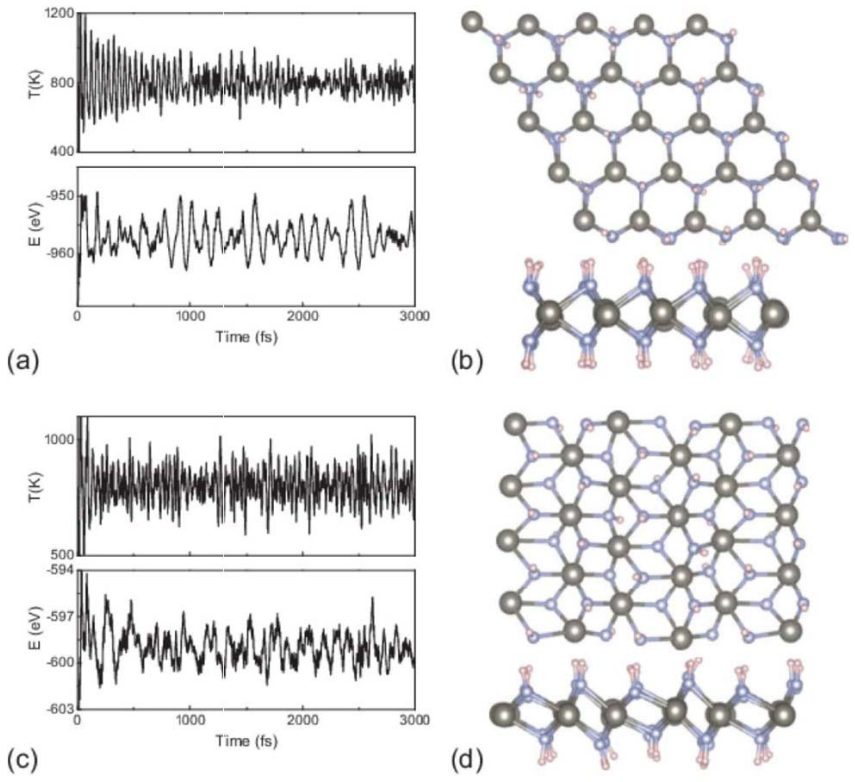

Figure S2. The fluctuations of temperature and free energy, as well as the final structures after the AIMD simulations for [(a), (b)] $H-WN_2H_2$ and [(c), (d)] $T_d-WN_2H_2$ sheets.

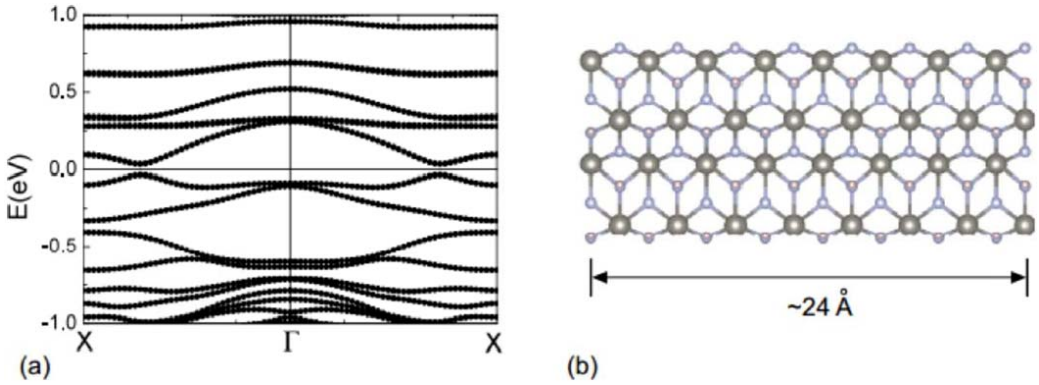

Figure S3. (a) The PBE+SOC bands and (b) atom structure of armchair T_d−WN_2H_2 nanoribbon.