Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Controllable P-type Doping of Monolayer MoS_2 with Tantalum by One-step Chemical Vapor Deposition

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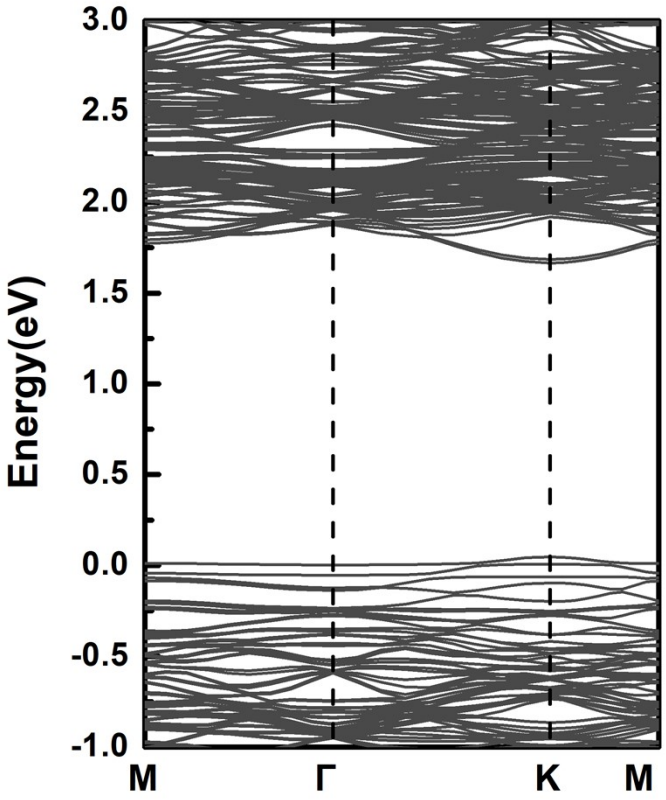

Figure S1. The electronic band structure of Ta-doped MoS_2 calculated by PBE with spin-orbit coupling (SOC).

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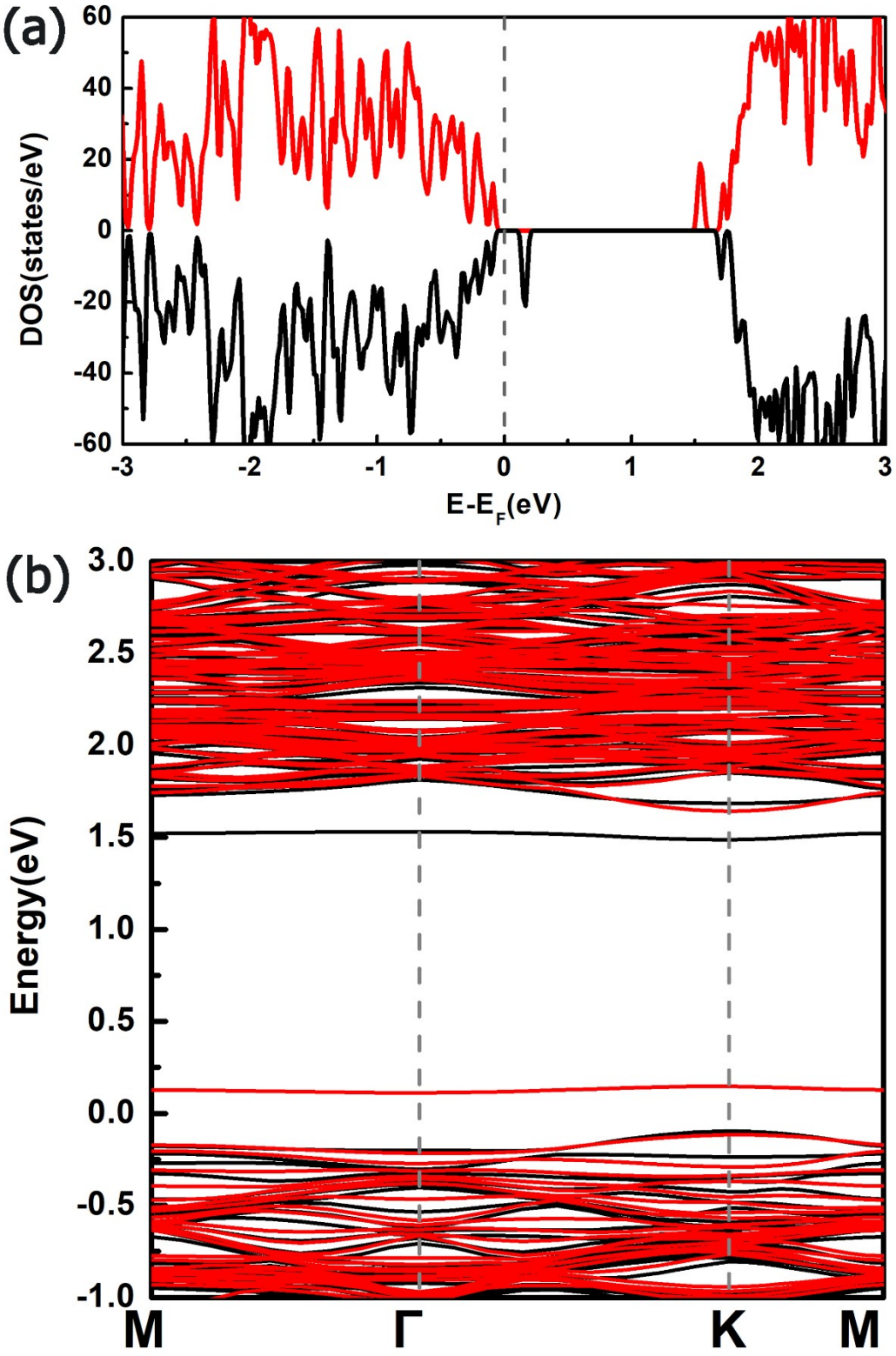

Figure S2. The electronic DOS and band structure of Ta-doped MoS_2 calculated by LDA+U functional based on DFT.

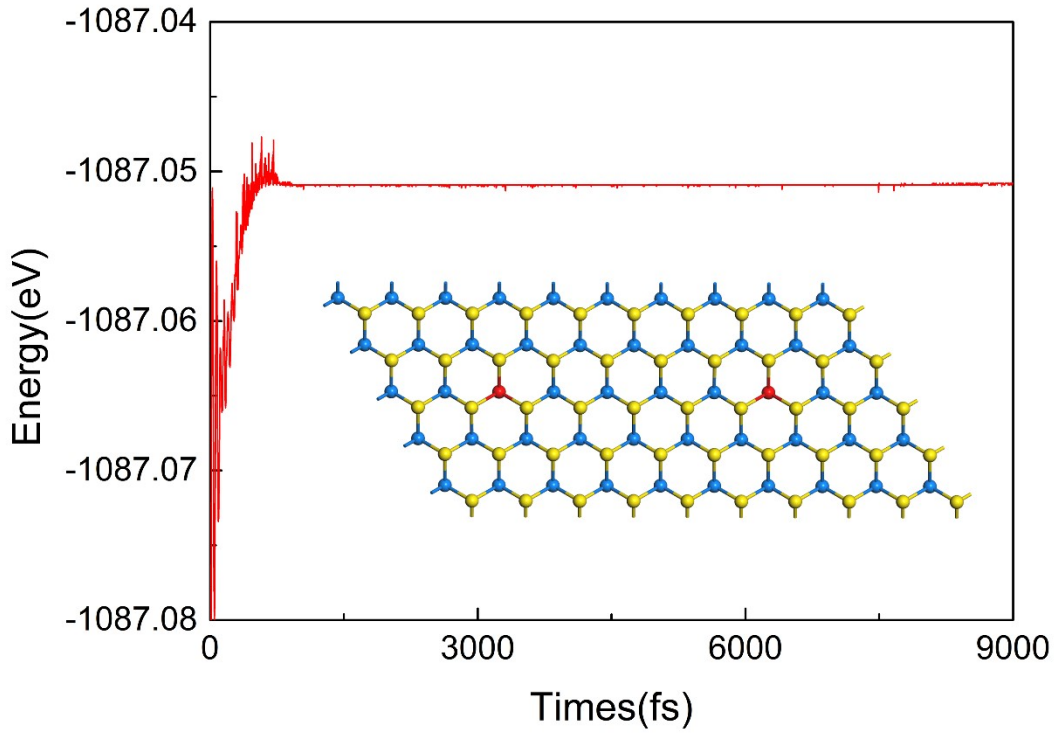

Figure S3. The thermodynamic property of Ta-doped MoS_2 calculated by molecular dynamics (MD) based on VASP with Andersen Thermostat set at 300K for the NVT ensemble.