Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Boosting the Hydrogen Evolution Reaction on NiTe Monolayer via the Defect Engineering: A Computational Study

Yuchen Xiang,[1] Yuting Sun,[1] Yuejie Liu,[2,*] Qinghai Cai,[1] Jingxiang Zhao[1,*]

[1] *College of Chemistry and Chemical Engineering, and Key Laboratory of Photonic and Electronic Bandgap Materials, Ministry of Education, Harbin Normal University, Harbin, 150025, China*

[2] *Modern Experiment Center, Harbin Normal University, Harbin 150025, China*

[*] *To whom correspondence should be addressed. Email: liuyuejie@hrbnu.edu.cn (Y. Liu); zhaojingxiang@hrbnu.edu.cn (J. Zhao)*

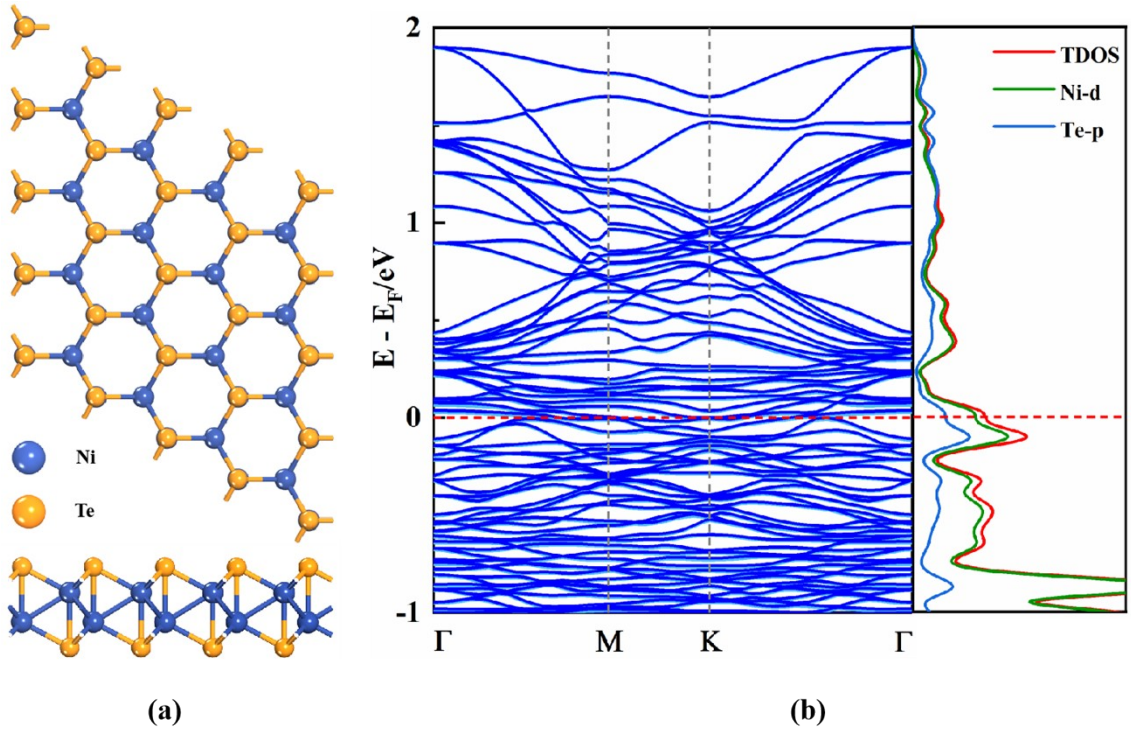

Fig. S1. (a) The top and side views and (b) the computed band structure and density of state (PDOS) for NiTe monolayer. The Fermi level was set to zero in red dashed line.

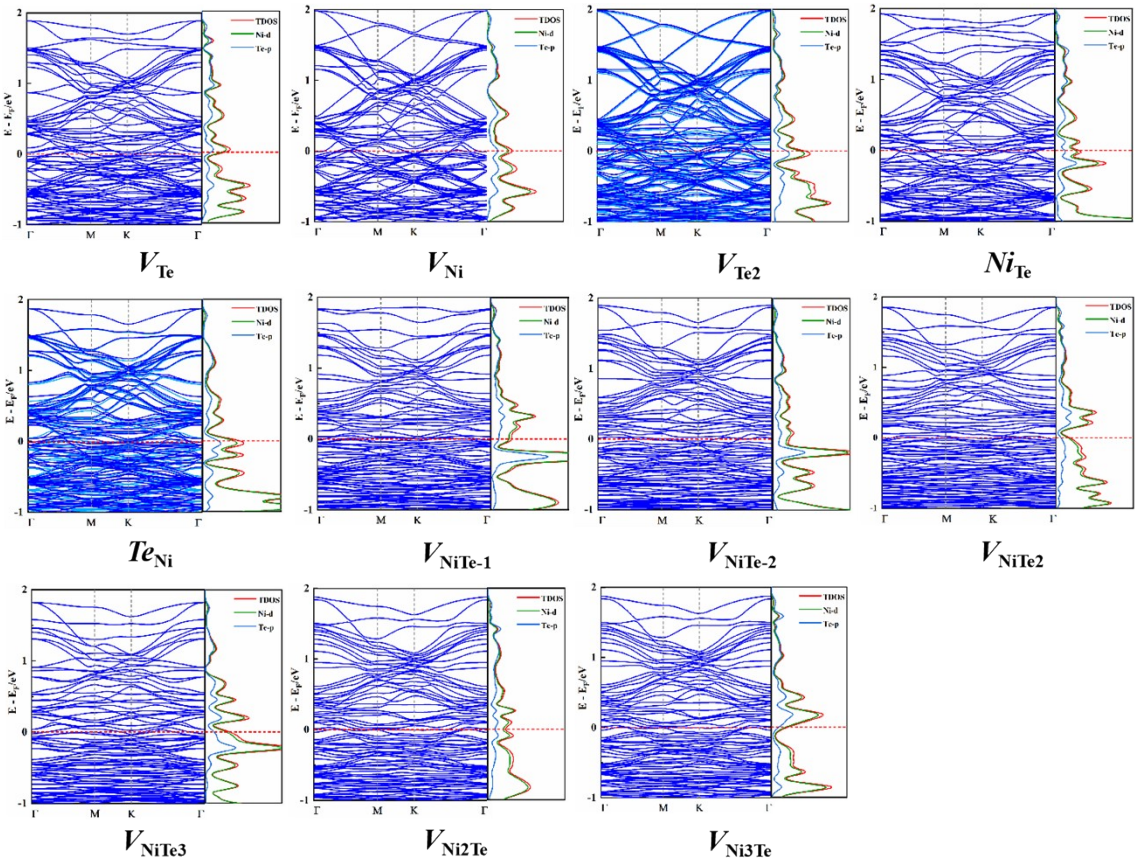

Fig. S2. The computed band structures and density of states (PDOSs) for different defective NiTe nanosheets. The Fermi level was set to zero in red dashed line.

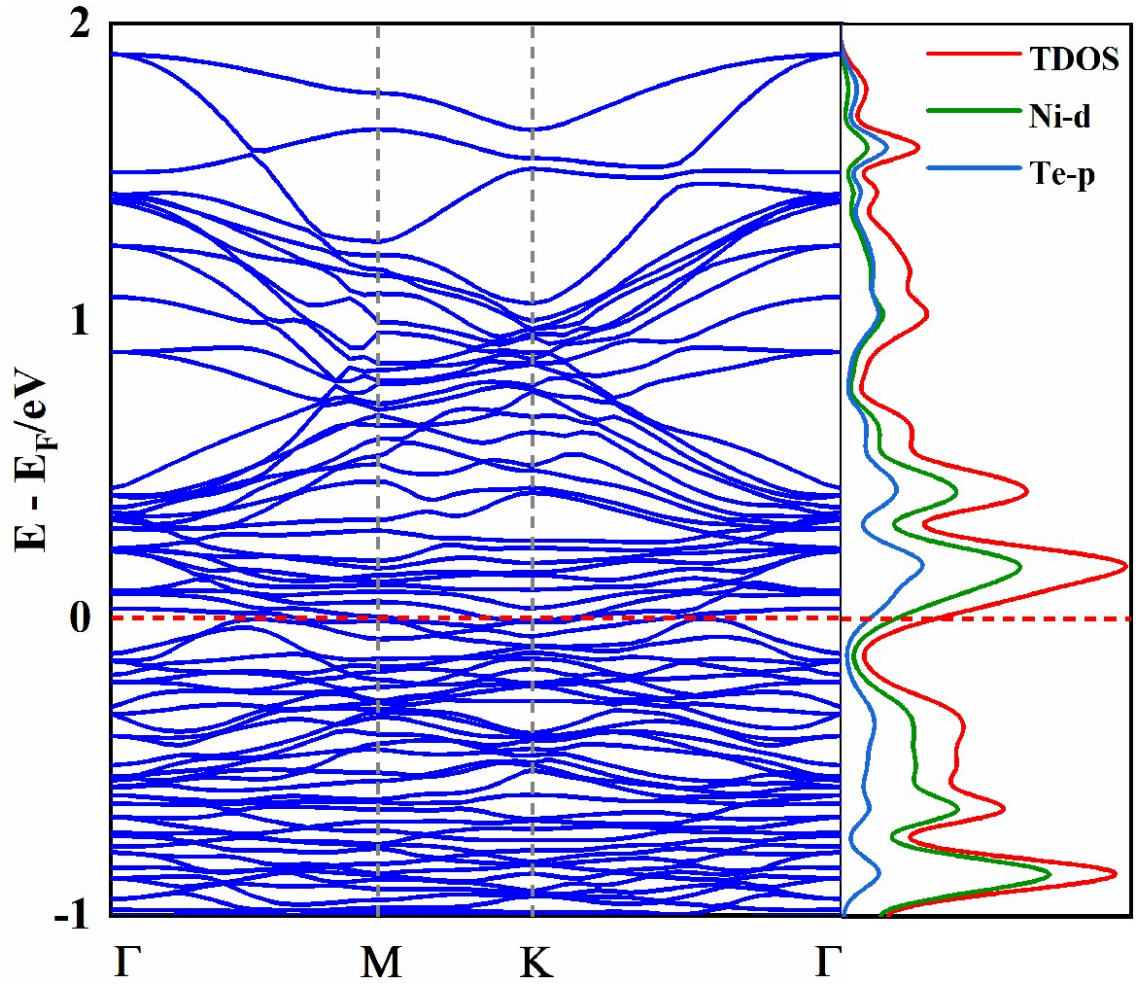

Fig. S3. The computed band structures and density of states (PDOSs) for V_{Ni3Te} system.

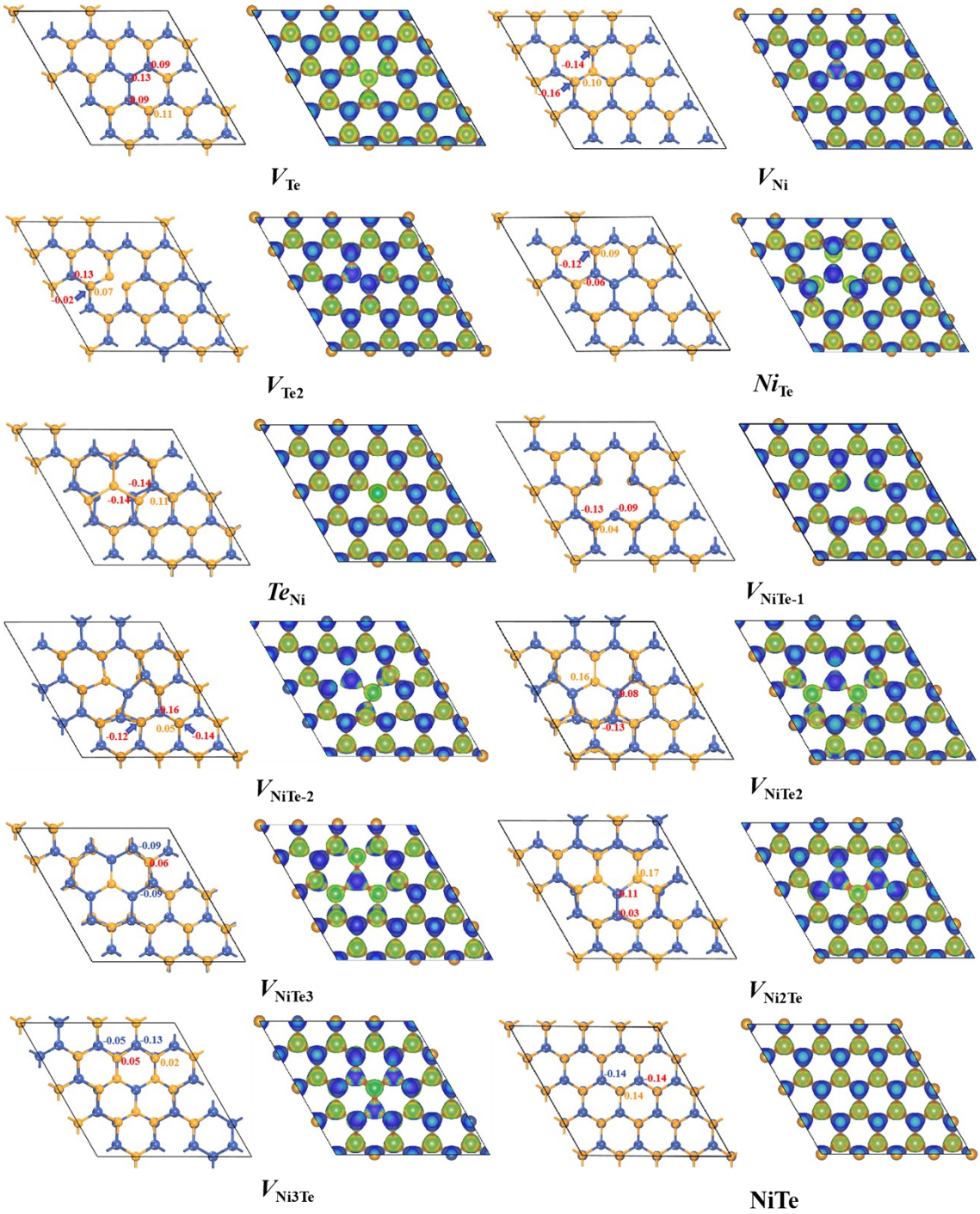

Fig. S4. The computed charge population and charge density of different defective NiTe nanosheets and pristine NiTe monolayer.

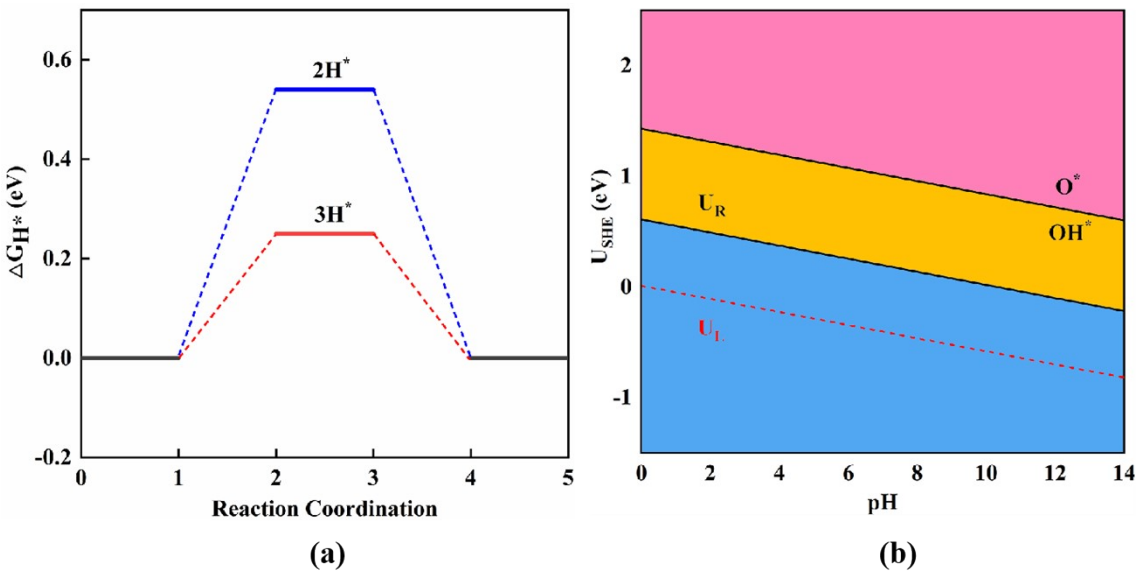

Fig. S5. (a) The computed ΔG_{H^*} values for V_{Ni3Te} system at the H^* high coverage and (b) Surface Pourbaix diagram of V_{Ni3Te}.

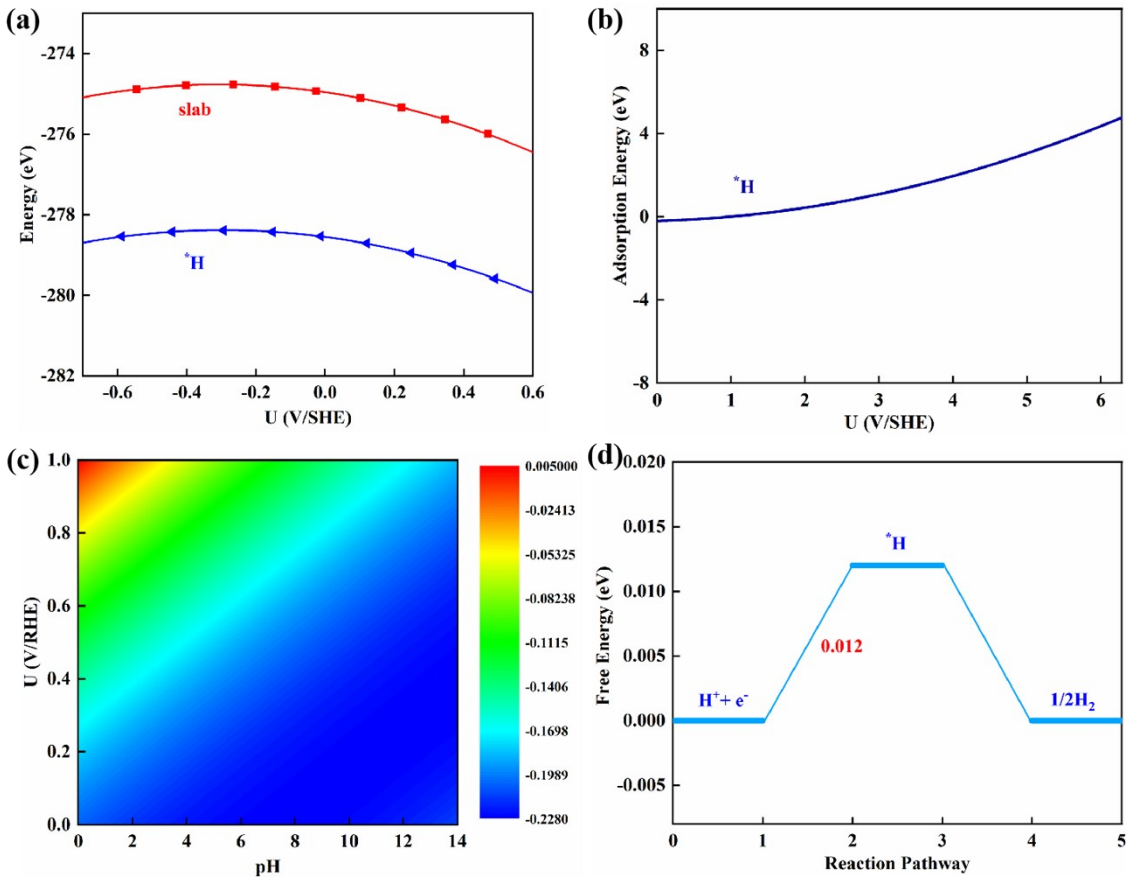

Fig. S6. (a) Computed energies of the V_{Ni3Te} and the corresponding reaction intermediates as a function of the applied electrode potential. (b) Adsorption energies of H^* as a function of the applied electrode potential. (c) pH-Dependent and potentialdependent contour plot of adsorption energies of H^* on the V_{Ni3Te}. (d) The free energy profile for H^* electrocatalytic reduction on the V_{Ni3Te} system in pH = 7.52.

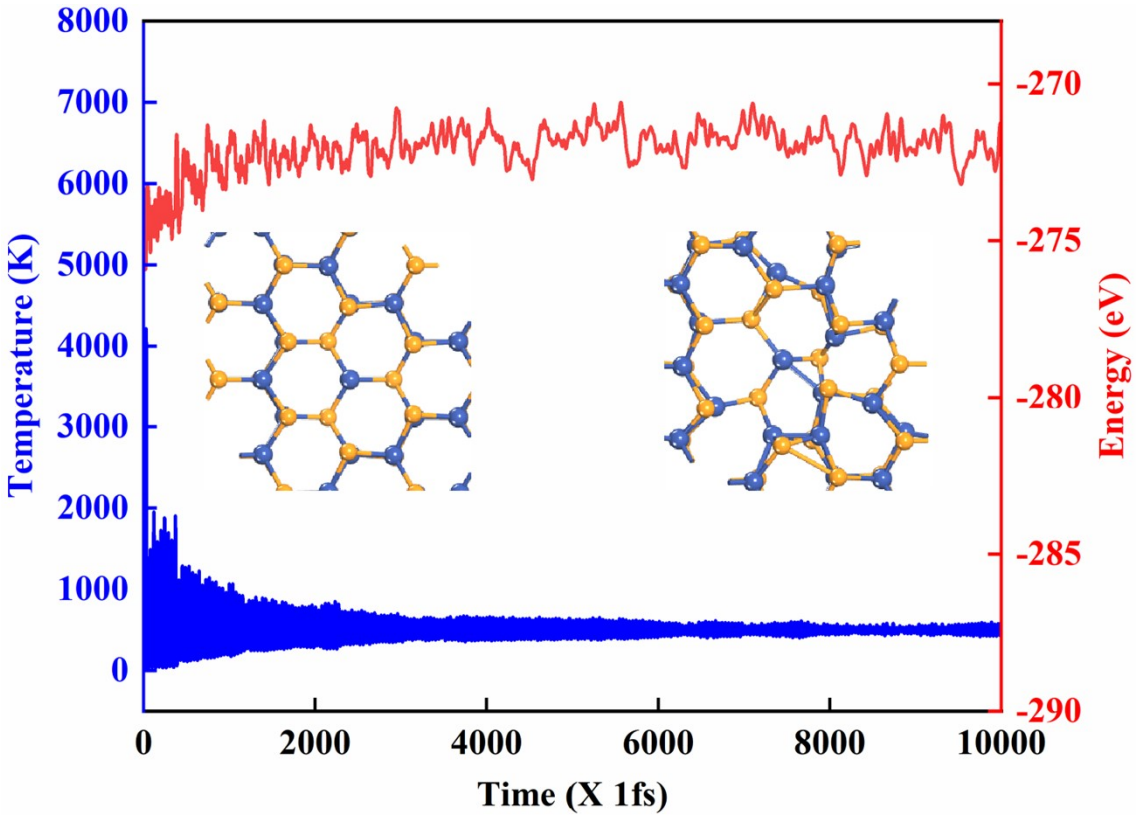

Fig. S7. Structure of V_{Ni3Te} monolayer after AIMD simulations at 500 K for a period of 10 ps with a time step of 1.0 fs, and the corresponding variations of temperature and energy versus simulation time.