Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Data

Effect of vacancy defects on the electromechanical properties of monolayer $NiTe_2$ monolayers from first principles

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Optimized structural coordinates of pristine monolayer 1T-$NiTe_2$

CELL PARAMETERS (angstrom)

3.806267222	0.000000000	0.000000000
-1.903133607	3.296320913	0.000000000
0.000000000	0.000000000	21.000000000

ATOMIC POSITIONS (angstrom)

Ni	0.0000000000	0.0000322117	6.2973831511
Te	0.0000015671	2.1975798630	4.9384007687
Te	1.9031356804	1.0988050501	7.6565525903

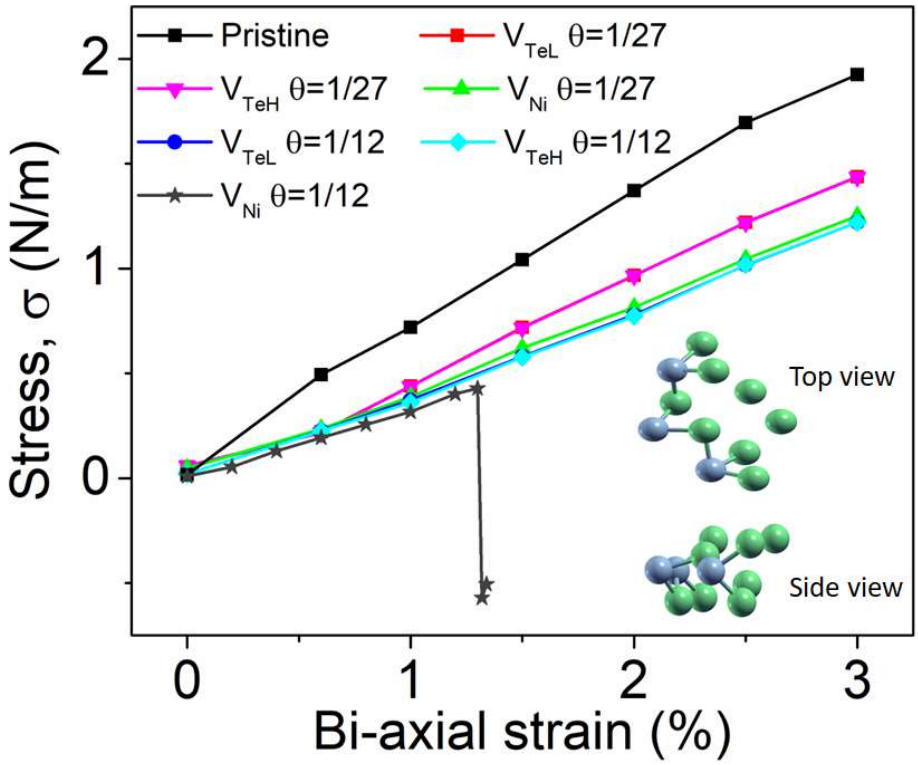

Fig. S1. Stress-strain curve of the pristine 1T-$NiTe_2$ monolayer and the 1T-$NiTe_2$ monolayers with Ni or Te vacancies. Inset is the deformed crystal structure of the monolayer 1T-$NiTe_2$ with V_{Ni} θ = 1/12 under the influence of bi-axial strain of 1.32%.

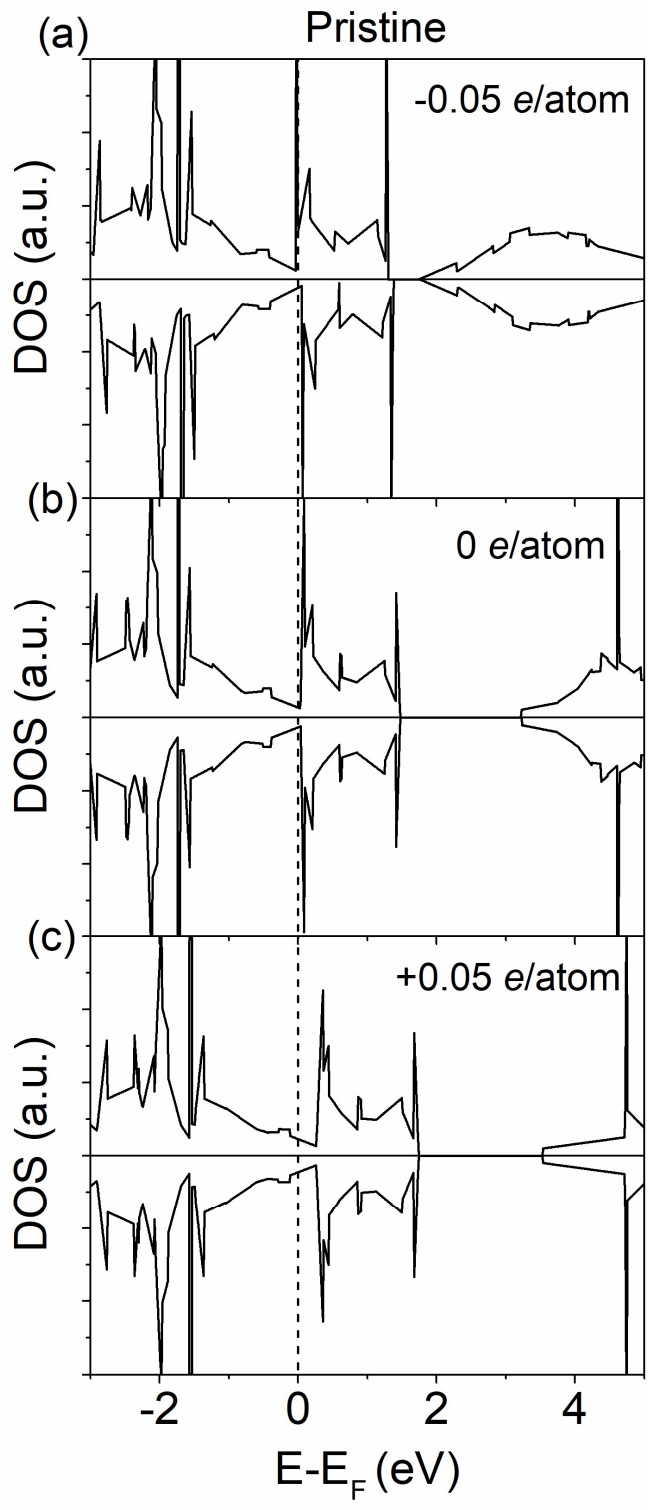

Fig. S1. Density of states (DOS) of pristine monolayer 1T-$NiTe_2$ for (a) q = -0.05 *e*/atom, (b) q = 0 *e*/atom and (c) q = +0.05 *e*/atom.

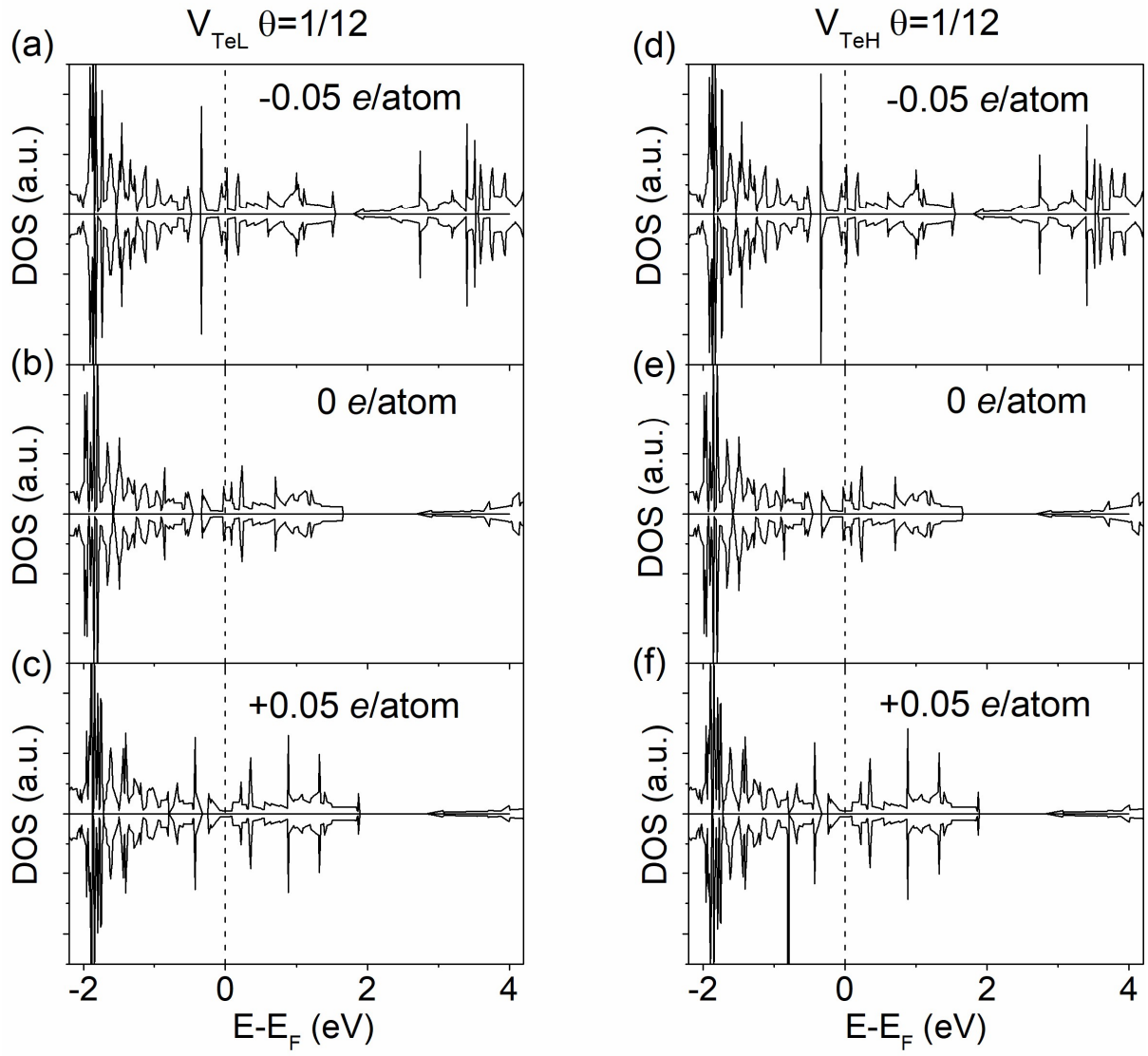

Fig. S3. Density of states (DOS) of the 1T-$NiTe_2$ monolayer with defects in the form of (a), (b), (c) V_{TeL} at $\theta = 1/12$ and (d), (e), (f) V_{TeH} at $\theta = 1/12$.

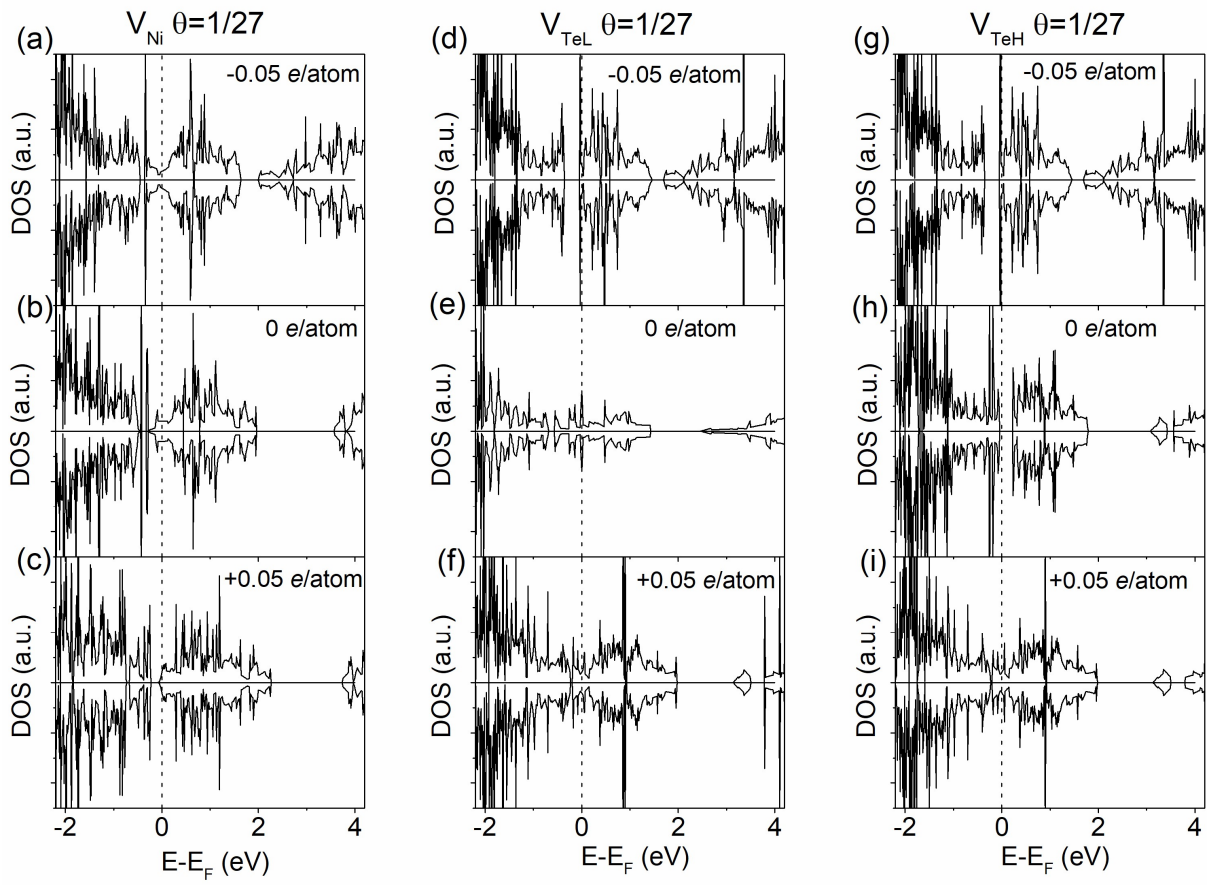

Fig. S4. Density of states (DOS) of the 1T-$NiTe_2$ monolayer with defects in the form of (a), (b), (c) V_{Ni} at θ = 1/27, (d), (e), (f) V_{TeL} at θ = 1/27 and (g), (h), (i) V_{TeH} at θ = 1/27

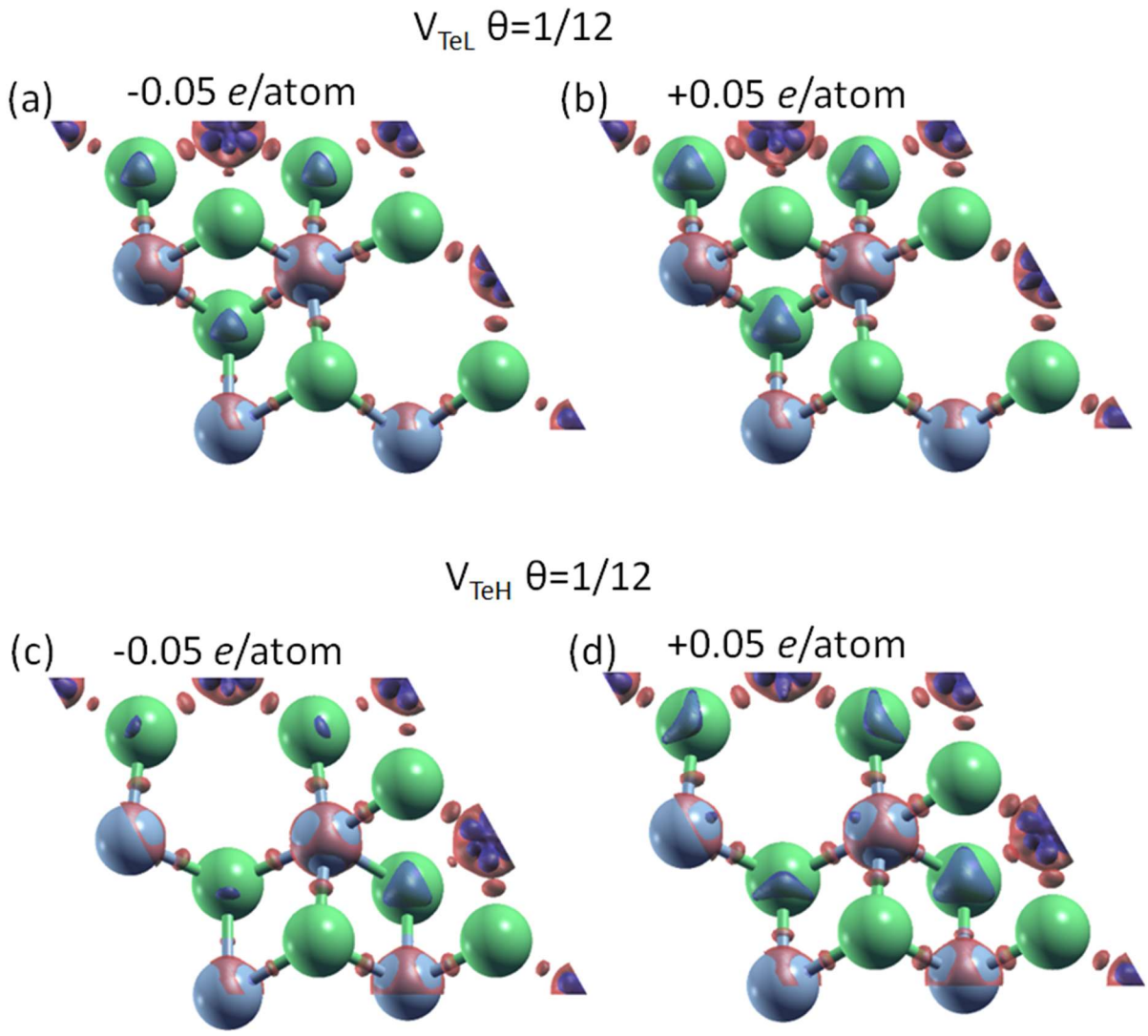

Fig. S5. The charge density difference between the monolayer 1T-$NiTe_2$ with V_{TeL} and V_{TeH} at θ = 1/12 and the superposition of the isolated atomic densities. The charge injection, *q* for (a) and (c) is -0.05 *e*/atom and for (b) and (d) is +0.05 *e*/atom. Red (blue) shaded region denotes the electron accumulation (depletion) region. The iso-surface is set at 0.009 *e*/bohr^3. The green and bluish balls represent Te and Ni atoms, respectively.

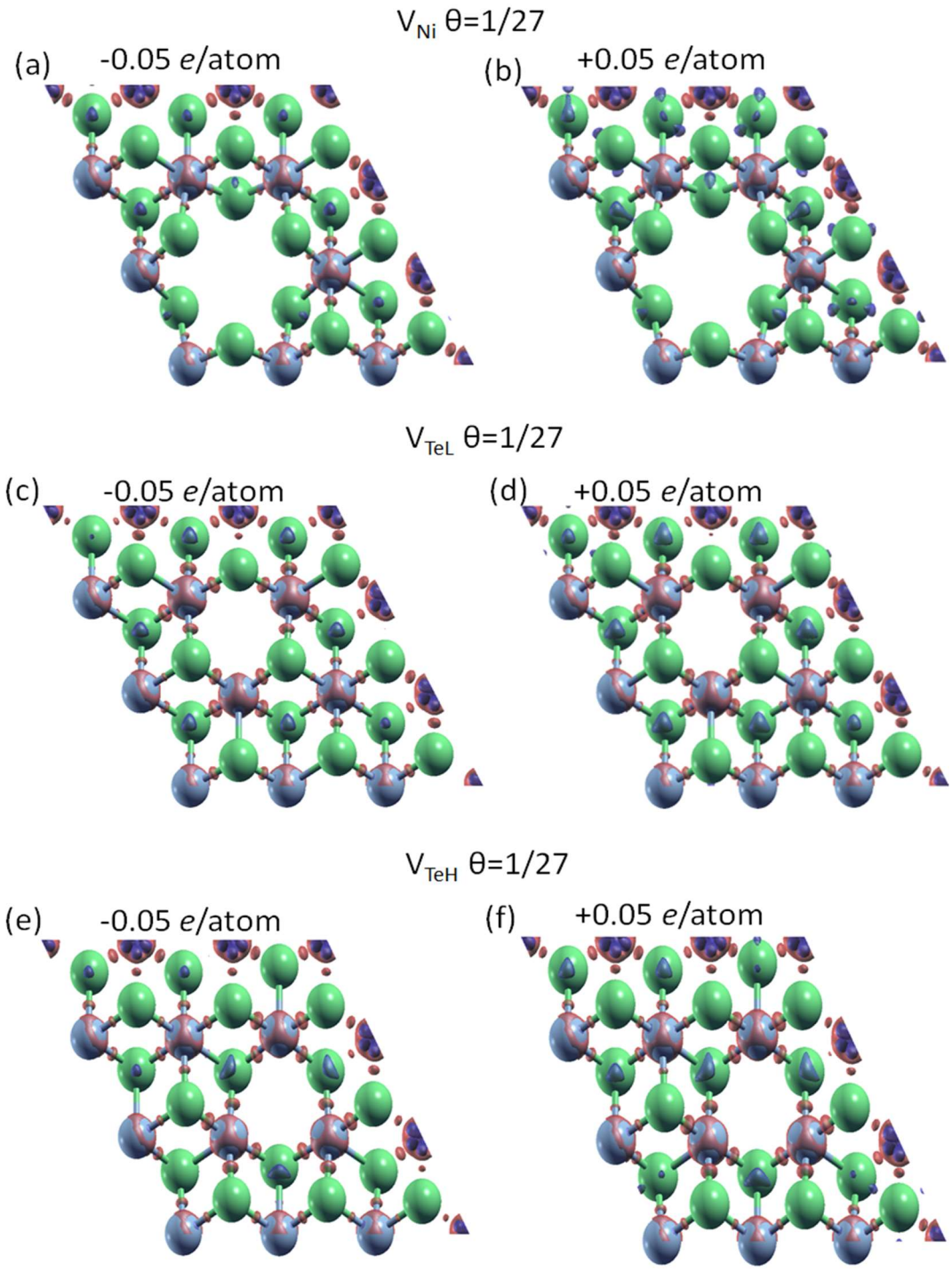

Fig. S6. The charge density difference between the monolayer 1T-$NiTe_2$ with V_{Ni}, V_{TeL} and V_{TeH} at θ = 1/27 and the superposition of the isolated atomic densities. The charge injection, *q* for (a), (c) and (e) is -0.05 *e*/atom and for (b), (d), (f) is +0.05 *e*/atom. Red (blue) shaded region denotes the electron accumulation (depletion) region. The iso-surface is set at 0.009 *e*/$bohr^3$. The green and bluish balls represent Te and Ni atoms, respectively.

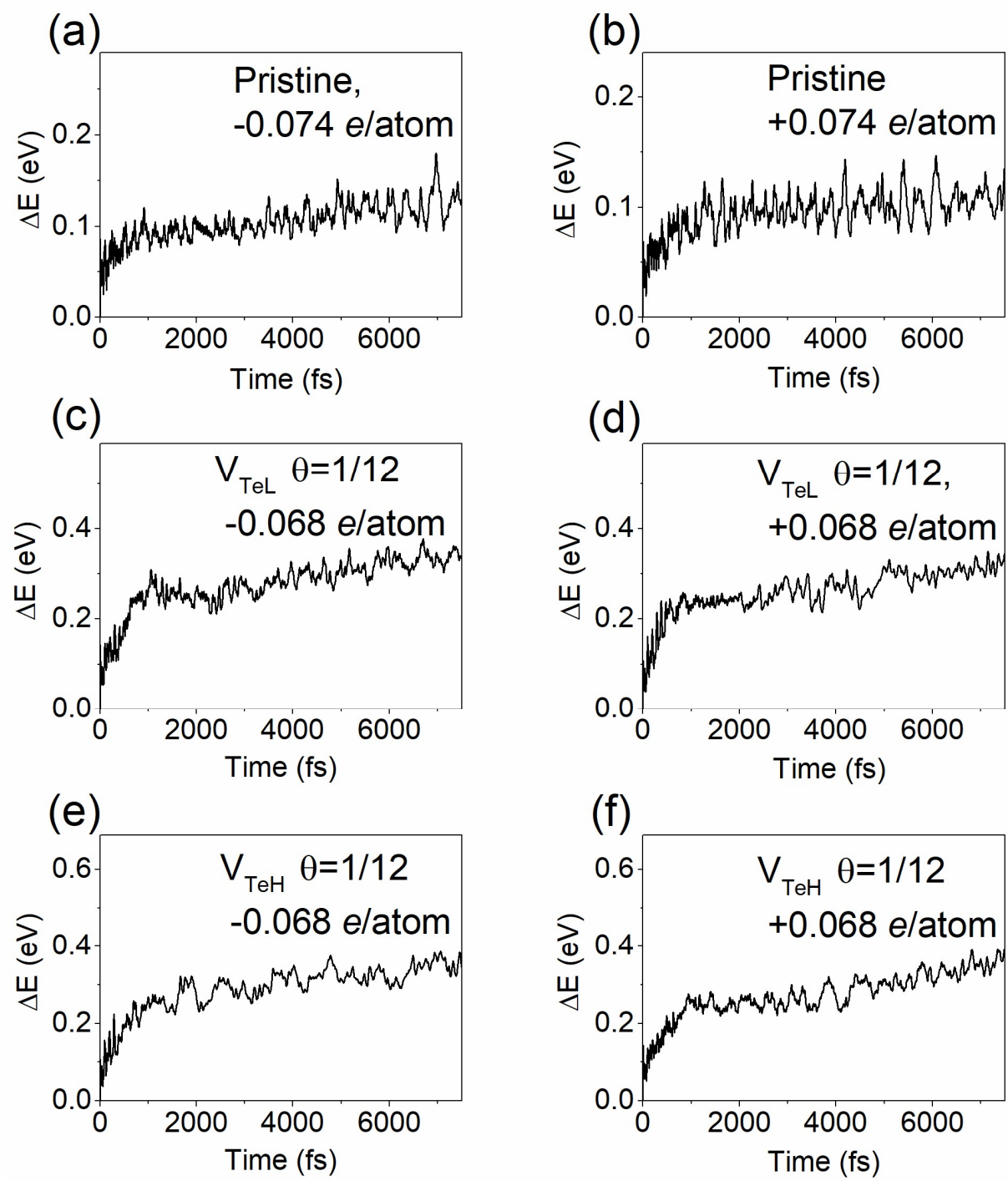

Fig. S7. Fluctuation of energy under AIMD simulations at 500 K for (a), (b) pristine monolayer 1T-$NiTe_2$, monolayer 1T-$NiTe_2$ with (c), (d) V_{TeL} at $\theta = 1/12$ (e), (f) V_{TeH} at $\theta = 1/12$. The evolution of the $NiTe_2$ crystal structures as a function of simulation time are provided in the movie clips

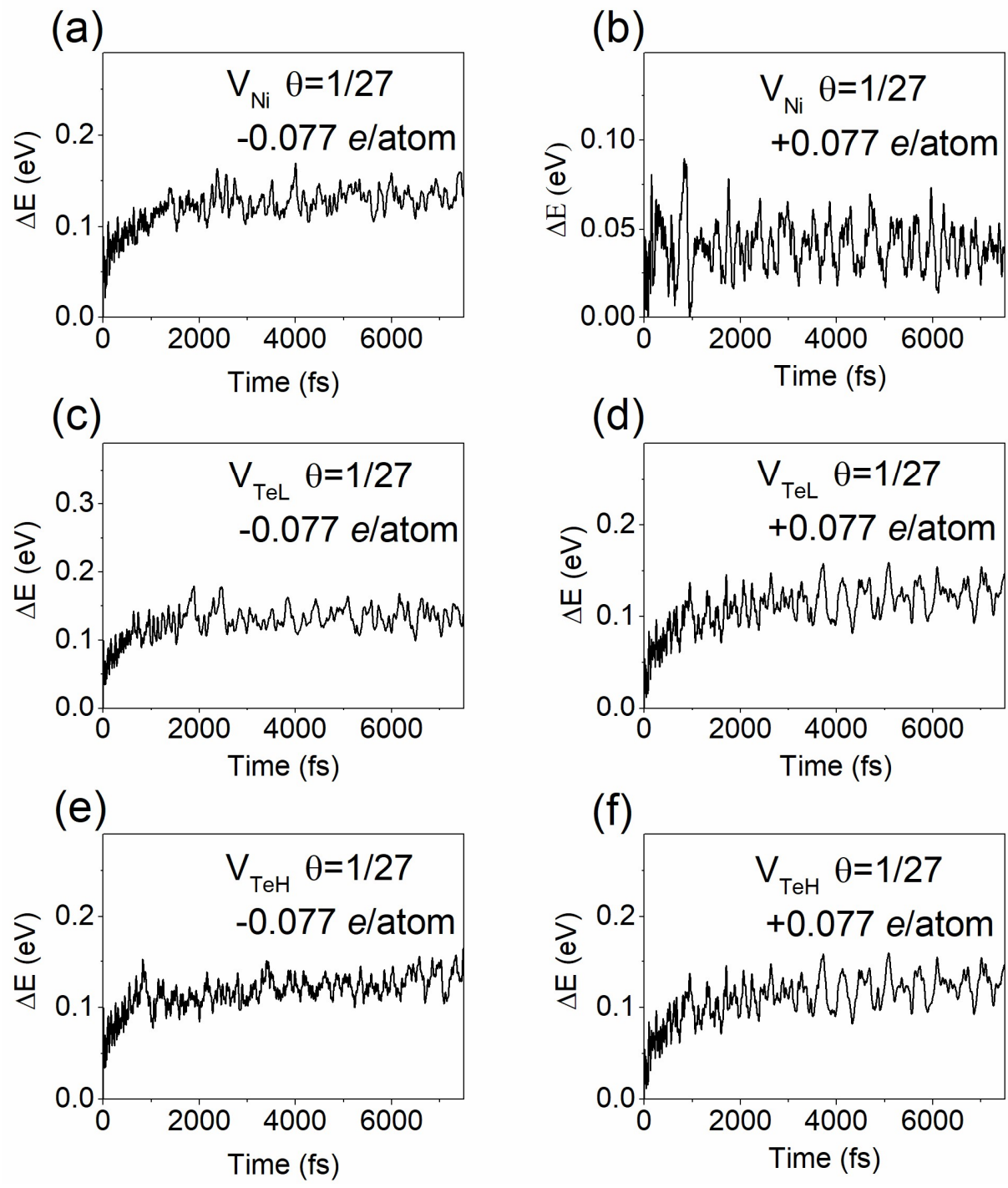

Fig. S8. Fluctuation of energy under AIMD simulations at 500 K for the monolayer 1T-$NiTe_2$ with (a), (b) V_{Ni} at $\theta = 1/27$, (c), (d) V_{TeL} at $\theta = 1/27$ and (e), (f) V_{TeH} at $\theta = 1/27$. The evolution of the $NiTe_2$ crystal structures as a function of simulation time are provided in the movie clips.

Table S1: Description of the movie clips provided in the Supplementary Data. These movie clips show the evolution of the $NiTe_2$ crystal structures as a function of AIMD simulation time at T=500K.

No.	File name	Description
1	Pristine.mpg	Pristine monolayer 1T-$NiTe_2$, q = 0 *e*/atom
2	Pristine-min.mpg	Pristine monolayer 1T-$NiTe_2$, q = -0.074 *e*/atom
3	Pristine-max.mpg	Pristine monolayer 1T-$NiTe_2$, q = +0.074 *e*/atom
4	2VTeL.mpg	Monolayer 1T-$NiTe_2$ with V_{TeL}, θ = 1/12, q = 0 *e*/atom
5	2VTeL-min.mpg	Monolayer 1T-$NiTe_2$ with V_{TeL}, θ = 1/12, q = -0.068 *e*/atom
6	2VTeL-max.mpg	Monolayer 1T-$NiTe_2$ with V_{TeL}, θ = 1/12, q = +0.068 *e*/atom
7	2VTeH.mpg	Monolayer 1T-$NiTe_2$ with V_{TeH}, θ = 1/12, q = 0 *e*/atom
8	2VTeH-min.mpg	Monolayer 1T-$NiTe_2$ with V_{TeH}, θ = 1/12, q = -0.068 *e*/atom
9	2VTeH-max.mpg	Monolayer 1T-$NiTe_2$ with V_{TeH}, θ = 1/12, q = +0.068 *e*/atom
10	3VNi.mpg	Monolayer 1T-$NiTe_2$ with V_{Ni}, θ = 1/27, q = 0 *e*/atom
11	3VNi-min.mpg	Monolayer 1T-$NiTe_2$ with V_{Ni}, θ = 1/27, q = -0.077 *e*/atom
12	3VNi-max.mpg	Monolayer 1T-$NiTe_2$ with V_{Ni}, θ = 1/27, q = +0.077 *e*/atom
13	3VTeL.mpg	Monolayer 1T-$NiTe_2$ with V_{TeL}, θ = 1/27, q = 0 *e*/atom
14	3VTeL-min.mpg	Monolayer 1T-$NiTe_2$ with V_{TeL}, θ = 1/27, q = -0.077 *e*/atom
15	3VTeL-max.mpg	Monolayer 1T-$NiTe_2$ with V_{TeL}, θ = 1/27, q = +0.077 *e*/atom
16	3VTeH.mpg	Monolayer 1T-$NiTe_2$ with V_{TeH}, θ = 1/27, q = 0 *e*/atom
17	3VTeH-min.mpg	Monolayer 1T-$NiTe_2$ with V_{TeH}, θ = 1/27, q = -0.077 *e*/atom
18	3VTeH-max.mpg	Monolayer 1T-$NiTe_2$ with V_{TeH}, θ = 1/27, q = +0.077 *e*/atom