Supplementary Information (SI) for Physical Chemistry Chemical Physics.

First-principles investigation on the corrosion resistance difference between the NiTi-B_2 and NiTi-B19' phases

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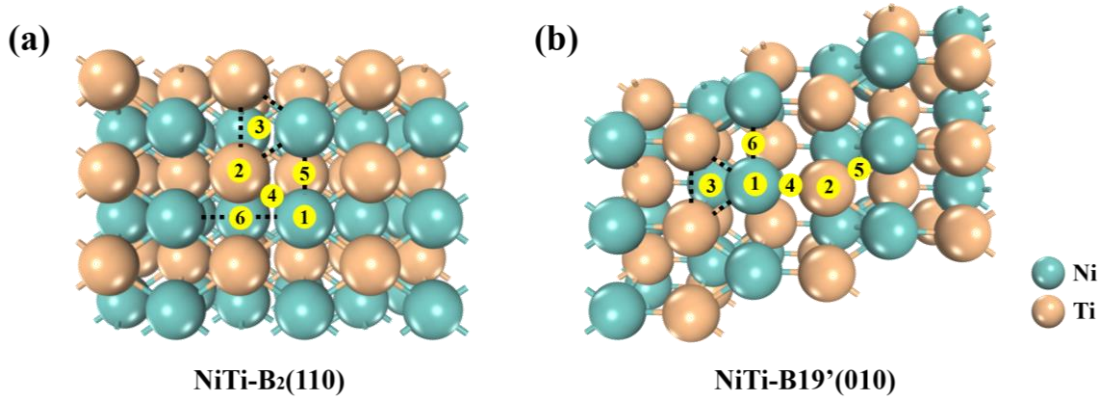

Fig. S1 Top views of the (a) NiTi-B_2(110) and (b) NiTi-B19'(010) surfaces with the following adsorption sites: 1 (above the Ni atom, referred to as Ni top), 2 (above the Ti atom, referred to as Ti top), and 3 (above a triangle formed by Ti and Ni atoms, hexagonal close-packed sites, referred to as Hcp). For the (a) NiTi-B_2(110) surface, sites labeled 4, 5, and 6 correspond to a bridge between Ni and Ti atoms (NiTi Bridge), a short bridge between two Ni atoms (NiNi Bridge-1), and a long bridge between two Ni atoms (NiNi-Bridge-2), respectively. For the (b) NiTi-B19'(010) surface, sites labeled 4 and 5 are bridges between Ni and Ti atoms (NiTi Bridge-1 and NiTi Bridge-2, respectively), and site 6 bridges between Ni atoms (NiNi Bridge). The solid yellow circle indicates the adsorption site.

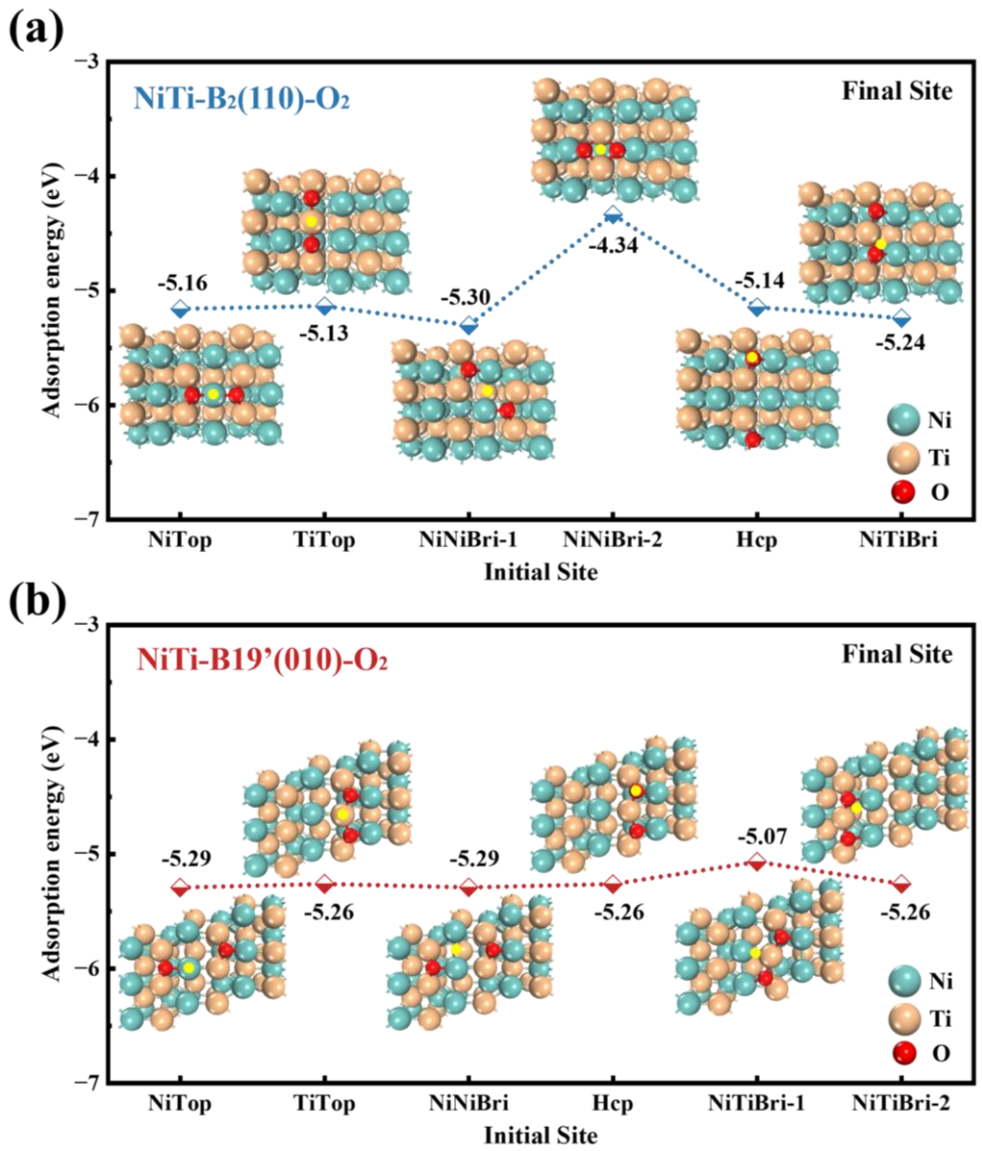

Fig. S2 Adsorption energy (E_{ads}) of one O_2 molecule on the NiTi-B_2(110) and NiTi-B19'(010) surface at varied sites as well as the corresponding stable adsorbed structure. The solid yellow circle indicates the initial site of the O_2 molecule. The E_{ads} of an O atom on each site was calculated using expression: $E_{ads} = \frac{1}{2}\left[E_{O_2/slab} - E_{slab} - E_{O_2}\right]$, where $E_{O_2/slab}$, E_{slab}, and E_{O_2} denote the total energy of the oxygen adsorbed slab, the slab before adsorption, and an isolated O_2 molecule, respectively.

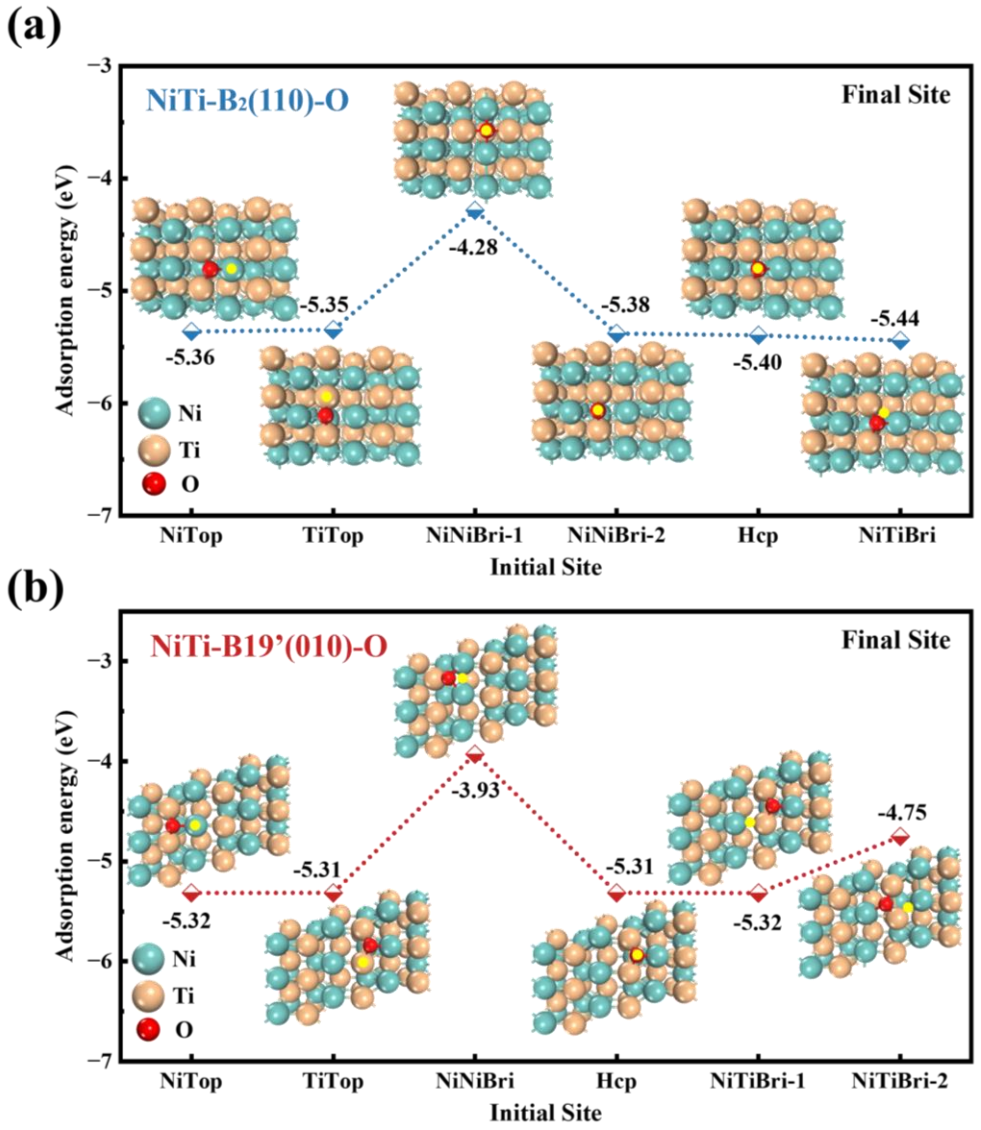

Fig. S3 Adsorption energy (E_{ads}) of an O atom on the NiTi-B_2(110) and NiTi-B19'(010) surfaces at varied sites as well as the corresponding stable adsorbed structure. The solid yellow circle indicates the initial site of the O atom.

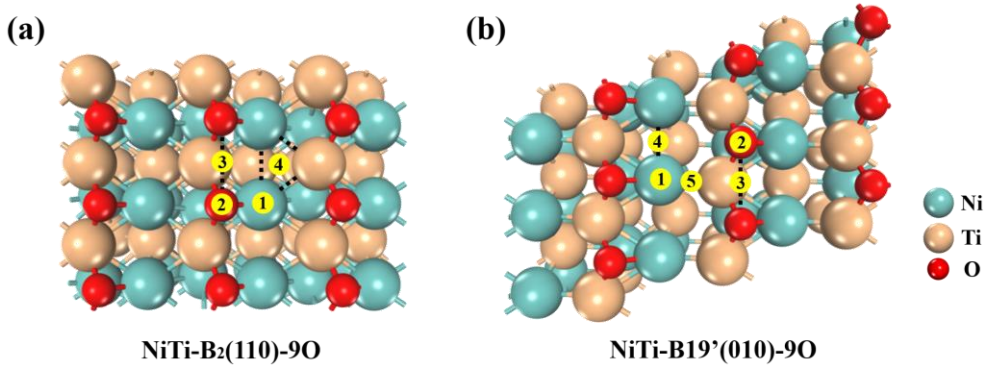

Fig. S4 Top views of the (a) NiTi-B_2(110)-9O and (b) NiTi-B19'(010)-9O surfaces with the following adsorption sites: 1 (above the Ni atom, namely, Ni top), 2 (above the O atom, namely, O top), and the sites labeled 3 correspond to a bridge between O and O atoms (namely, OO Bridge).

For the NiTi-B_2(110)-9O surface, the sites labeled 4 correspond to a triangle formed by Ti and Ni atoms, namely, Hcp. For the NiTi-B19'(010)-9O surface, the sites labeled 4 is bridge between Ni atoms, namely, NiNi Bridge; and the site labeled 5 is bridging between Ni and Ti atoms (namely, NiTi Bridge). The solid yellow circle indicates the adsorption site.

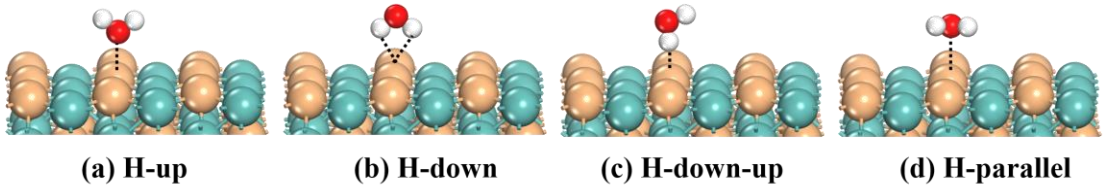

Fig. S5 H_2O molecule adsorbed at the Ti top site with four different initial orientations on the NiTi alloy surface. (a) H-up (H_2O molecular plane is normal to the alloy surface with two hydrogen atoms sitting at the same height, and two hydrogen atoms are above the oxygen atom), (b) H-down (two hydrogen atoms sit at the same height and below the oxygen atom), (c) H-down-up (only one of O-H bonds point to the alloy surface), and (d) H-parallel (H_2O molecular plane is normal to the alloy surface with two hydrogen atoms sitting at the same height).

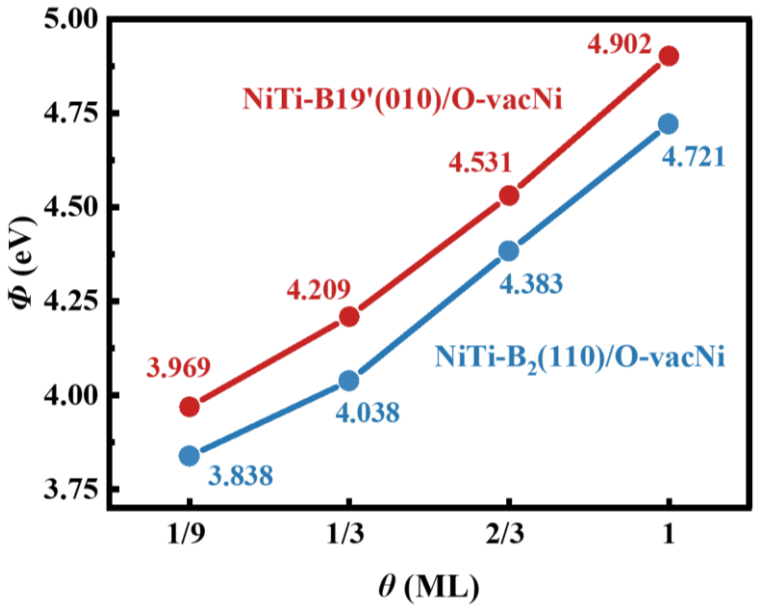

Fig. S6 Work functions (Φ) of the NiTi-B_2(110)/O-vacNi and NiTi-B19'(010)/O-vacNi surfaces at different θ.

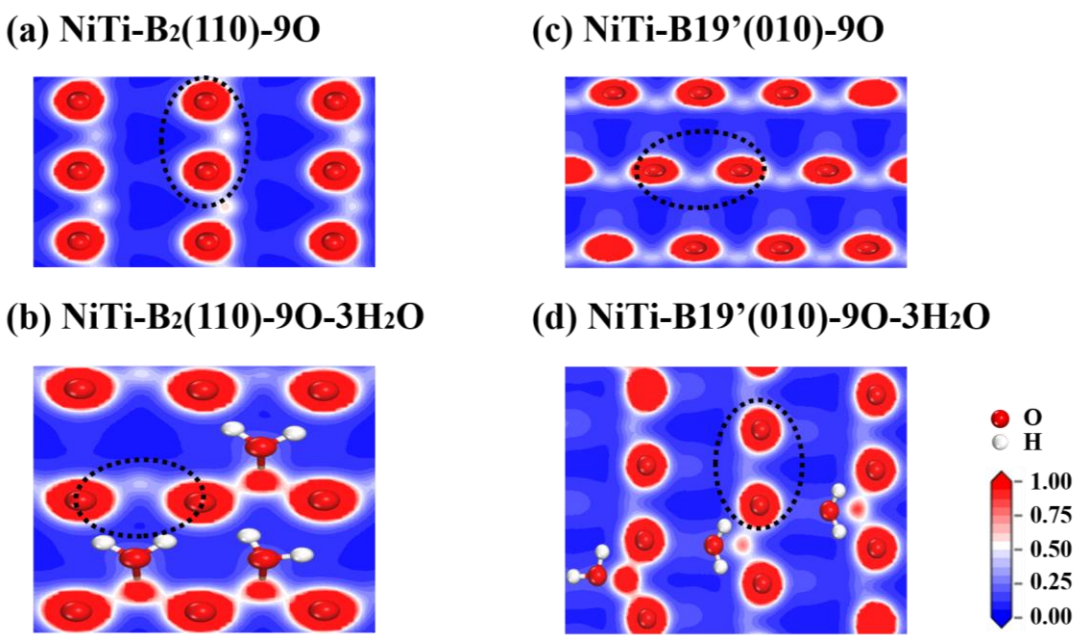

Fig. S7 Electron density analysis of the adsorption structures of O and H_2O on the NiTi alloy surfaces.

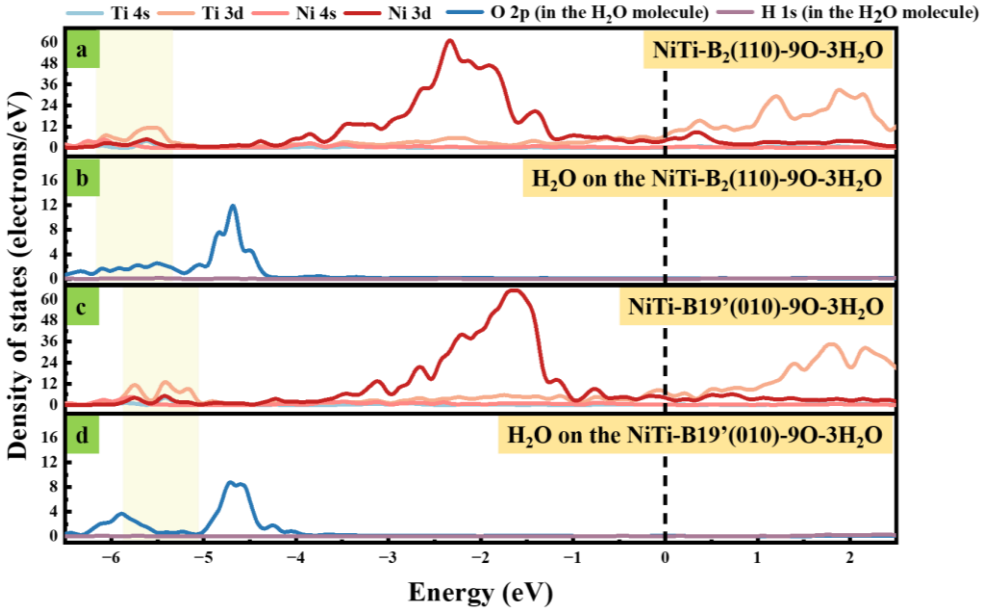

Fig. S8 Partial density of states (PDOS) between H_2O and surface Ti/Ni atoms on the NiTi alloy surfaces.

Table S1 The indirect interaction energy (E_{ind}) of O atoms adsorbed on the NiTi alloy surface for different θ.

θ (ML)	E_{ind} (eV)	
	NiTi-B_2(110)/O	NiTi-B19'(010)/O
1/9	—	—
1/3	-0.32	-0.07
2/3	-0.44	-0.19
1	-0.53	-0.23

Table S2 Surface vacancy formation energies (E_{form}^{vac}) of Ni or Ti vacancies on the clean NiTi-B_2(110) and NiTi-B19'(010) surfaces.

Type of slab	E_{vac} (eV)
NiTi-B_2(110)-vacNi	1.25
NiTi-B_2(110)-vacTi	1.06
NiTi-B19'(010)-vacNi	1.28
NiTi-B19'(010)-vacTi	1.12

Table S3 Adsorption energy ($E_{ads}(H_2O)$) of one H_2O molecule adsorption at varied sites on the clean NiTi-B_2(110) and NiTi-B19'(010) surfaces.

Type of slab	Initial site of H_2O	$E_{ads}(H_2O)$ (eV)	Final site of H_2O
NiTi-B_2(110)	Ni Top	-1.37	Ti Top
	Ti Top	-1.47	Ti Top
	NiNi Bri-1	-1.37	Ti Top
	NiNi Bri-2	-1.30	Ti Top
	Hcp	-1.37	NiNi Bri-2
	NiTi Bri	-1.42	Ti Top
NiTi-B19'(010)	Ni Top	-1.01	Ti Top
	Ti Top	-1.00	Ti Top
	NiNi Bri	-1.00	Ti Top
	Hcp	-1.03	Ti Top
	NiTi Bri-1	-1.00	Ti Top
	NiTi Bri-2	-1.02	Ti Top

Table S4 Adsorption energy ($E_{ads}(H_2O)$) of one H_2O molecule adsorption at varied sites on the NiTi-B_2(110)-9O and NiTi-B19'(010)-9O surfaces.

Type of slab	Initial site of H_2O	$E_{ads}(H_2O)$ (eV)	Final site of H_2O
NiTi-B_2(110)-9O	Ni Top	-1.17	Hcp
	O Top	-0.35	OO Bri
	OO Bri	-0.38	OO Bri
	Hcp	-1.18	Hcp
NiTi-B19'(010)-9O	Ni Top	-0.66	NiTi Bri
	O Top	-0.65	NiTi Bri
	OO Bri	-0.64	NiTi Bri
	NiNi Bri	-0.65	NiTi Bri
	NiTi Bri	-0.65	NiTi Bri