Bending-induced modulation doping: a promising tendency in silicon nanowires

Yuehan Li[a*], *Yue Zhang*[a*], *Suyang Zhang*[a], *Zun Xie*[†a] and *Zhao Liu*[‡a]

[a]Department of Physics and Hebei Advanced Thin Film Laboratory, Hebei Normal University, Shijiazhuang, 050024, China

[†]Corresponding author: zxie@hebtu.edu.cn

[‡]Corresponding author: zliu@hebtu.edu.cn

[*] These authors contributed equally.

S1. Doping preference for [001]-oriented tetrahedral SiNW.

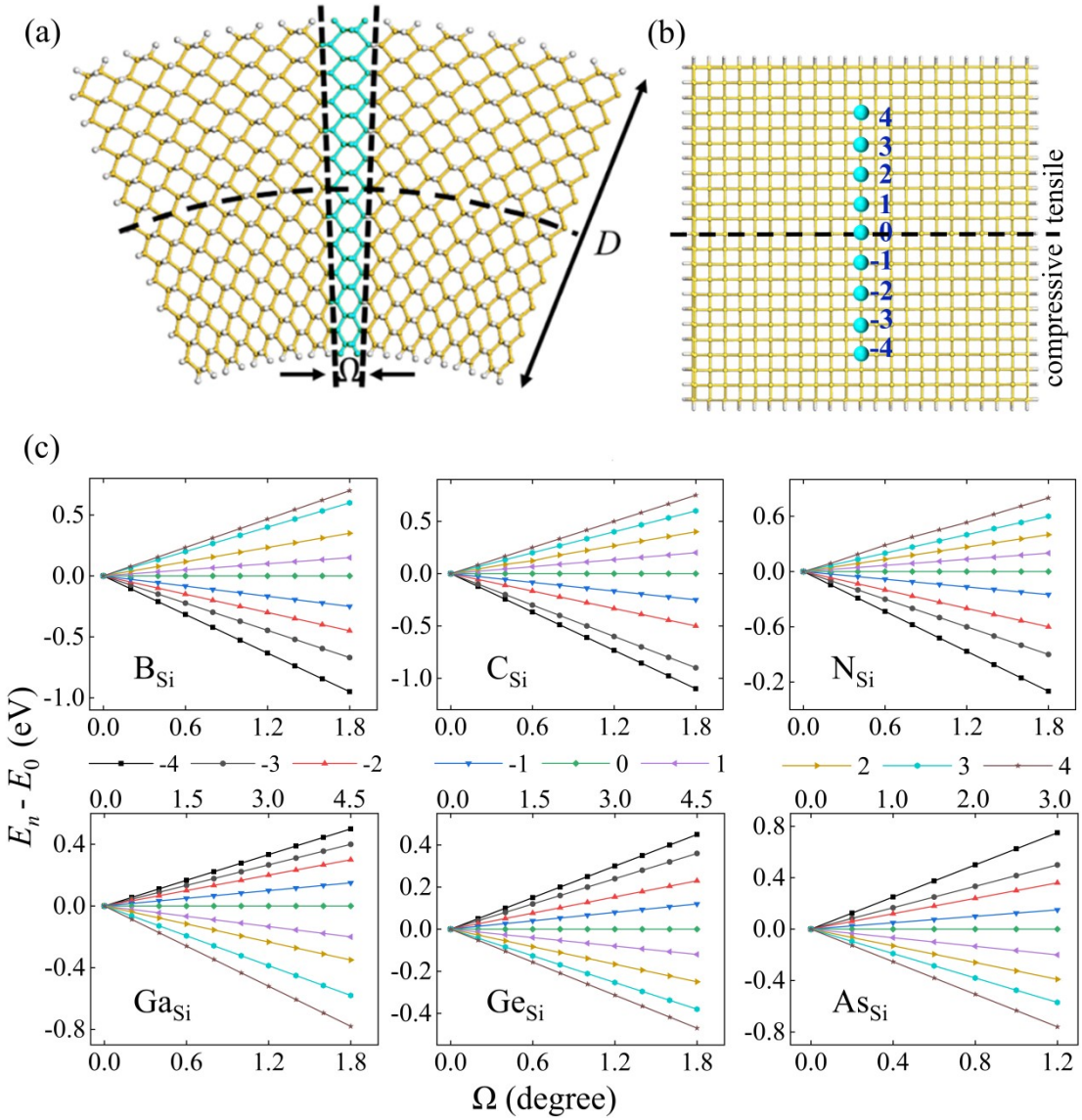

FIG. S1 (a) A side view of a bent tetrahedral SiNW along the [111] growth direction, with a diameter ***D*** = 4.22 nm. Ω represents the bending angle, and the dashed arc indicates the strain-free neutral surface. The primitive motif used in calculation is shown in green. (b) A cross-section of the SiNW depicted in (a), with 9 doping sites (red balls): sites n = 1, 2, 3, 4 are on the tensile side, sites n = -1, -2, -3, -4 are on the compressive sidere on the compressive side, site n = 0 is on the neutral surface. (c) The relative formation energy $E_n - E_0$ at site n versus

the bending angle Ω. X_{Si} (X = B, C, N, Ga, Ge, As) denotes the doping cases where the host Si atom is substituted with the dopant X atom.

S2. Energy bands and carrier distributions for [001]-oriented SiNW

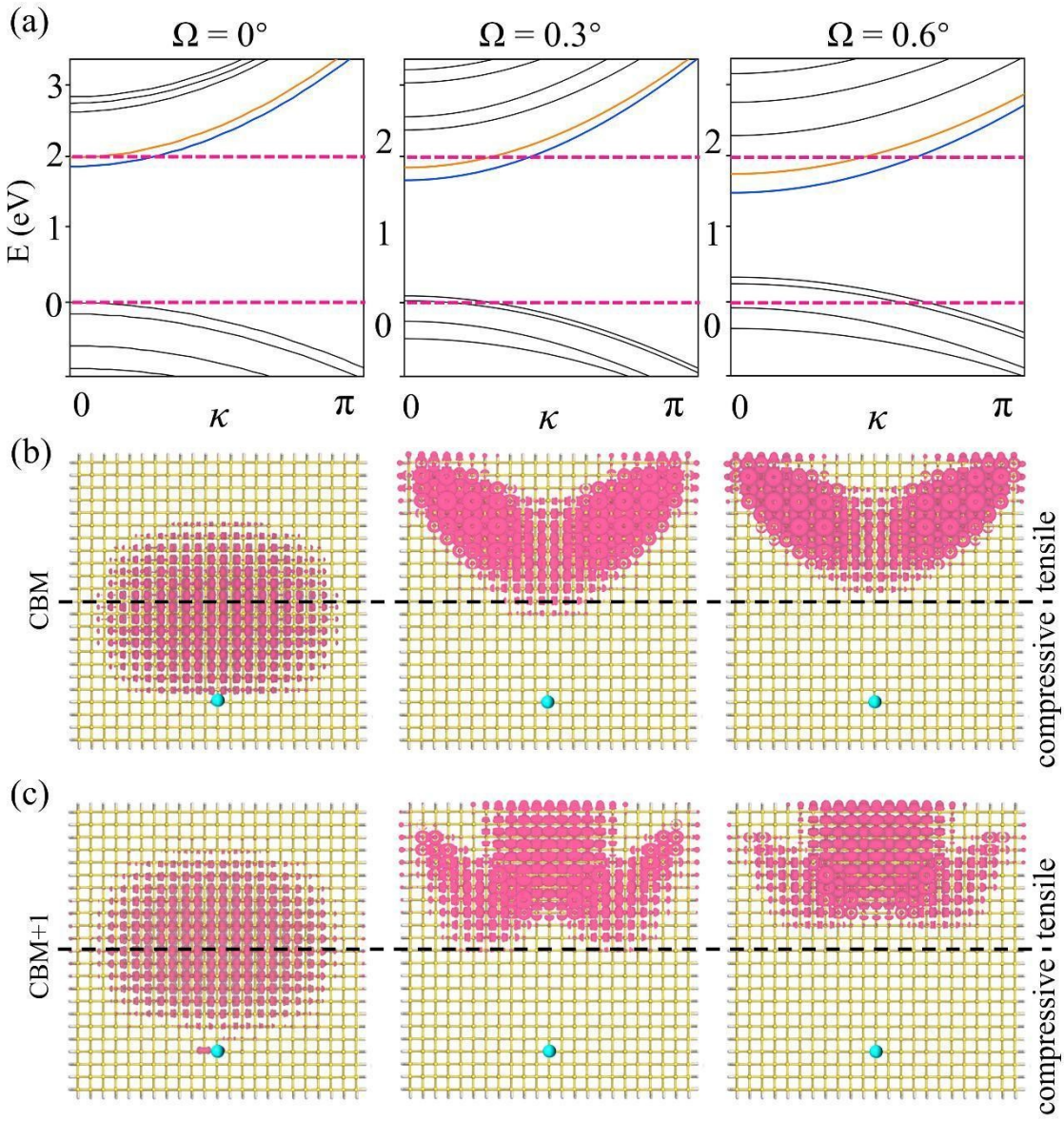

FIG. S2 [001]-oriented SiNW with a diameter of ***D*** = 4.22 nm after N doped at position n = -4. (a) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3°and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (c) the CBM+1 state, where the CBM state corresponds to the blue line in Fig. S2(a) and the CBM+1 state corresponds to the orange line in Fig. S2(a). Dopants are represented by blue spheres. The isosurface level is 1.72×10^{-6} e Å^{-3}.

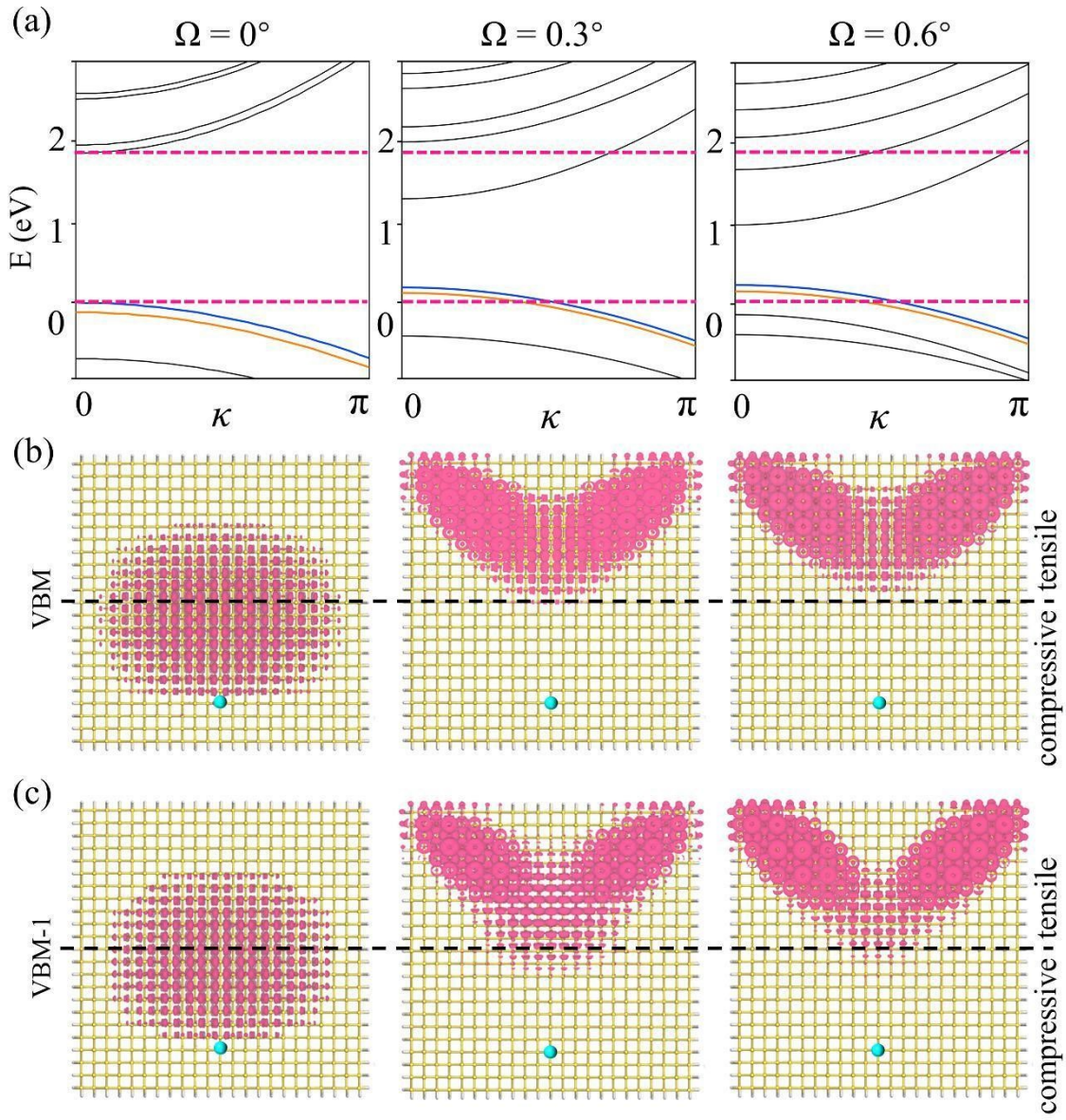

FIG. S3 [001]-oriented SiNW with a diameter of ***D*** = 4.22 nm after B doped at position n = -4. (a) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3°and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) VBM state and (c) the VBM-1 state, where the VBM state corresponds to the blue line in Fig. S3(a) and the VBM-1 state corresponds to the orange line in Fig. S3(a). Dopants are represented by blue spheres. The isosurface level is 1.72×10^{-6} e Å^{-3}.

S3. Band structure for bulk Si.

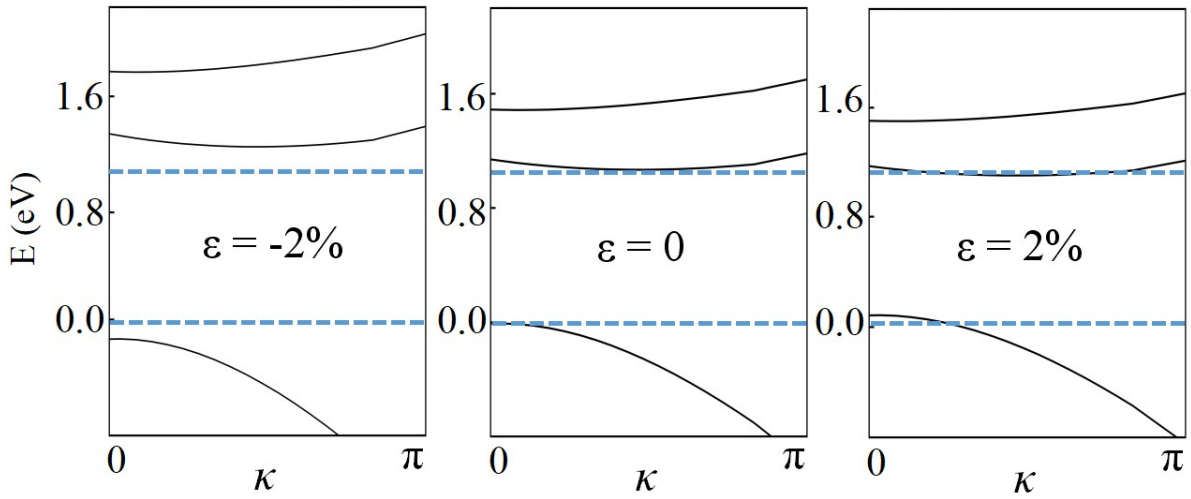

FIG. S4 Energy band of bulk Si with uniaxial tension and compression along the [001] direction of the SiNW.

S4. The comparison between DFTB+ and DFT data.

System	Method	Band gap (eV)
bulk Si	DFTB+	1.31
	GGA	0.607[1]
	BLYP	1.39[2]
	BPBE	1.13[2]
	Exp.	~1.17[3]

Table S1 The calculated band gaps with different methods of bulk silicon.

System	Diameter (nm)	Band gap (eV)	Ref. Band gap (eV)
[111] Si NW	0.92	2.85	2.25[4]
	1.69	2.21	1.34[4]
	2.46	2.04	1.13[4]
[011] Si NW	1.2	2.14	1.51[4]
	2.2	1.77	0.89[4]
	3.3	1.55	0.78[4]
[001] Si NW	1.1	3.23	2.35[5]
	2.0	2.58	1.32[5]

Table S2 The calculated band gaps comparison of SiNWs along different orients.

[1]Crystals **14**, 585 (2024).

[2]Phys. Rev. B **76**, 155435 (2007).

[3] Solid State Phys. **1**, 2 (1976).

[4]Phys. Rev. B **74**, 045116 (2006).

[5]Phys. Rev. Lett. **92**, 236805 (2004).

S5. Calculations with supercell.

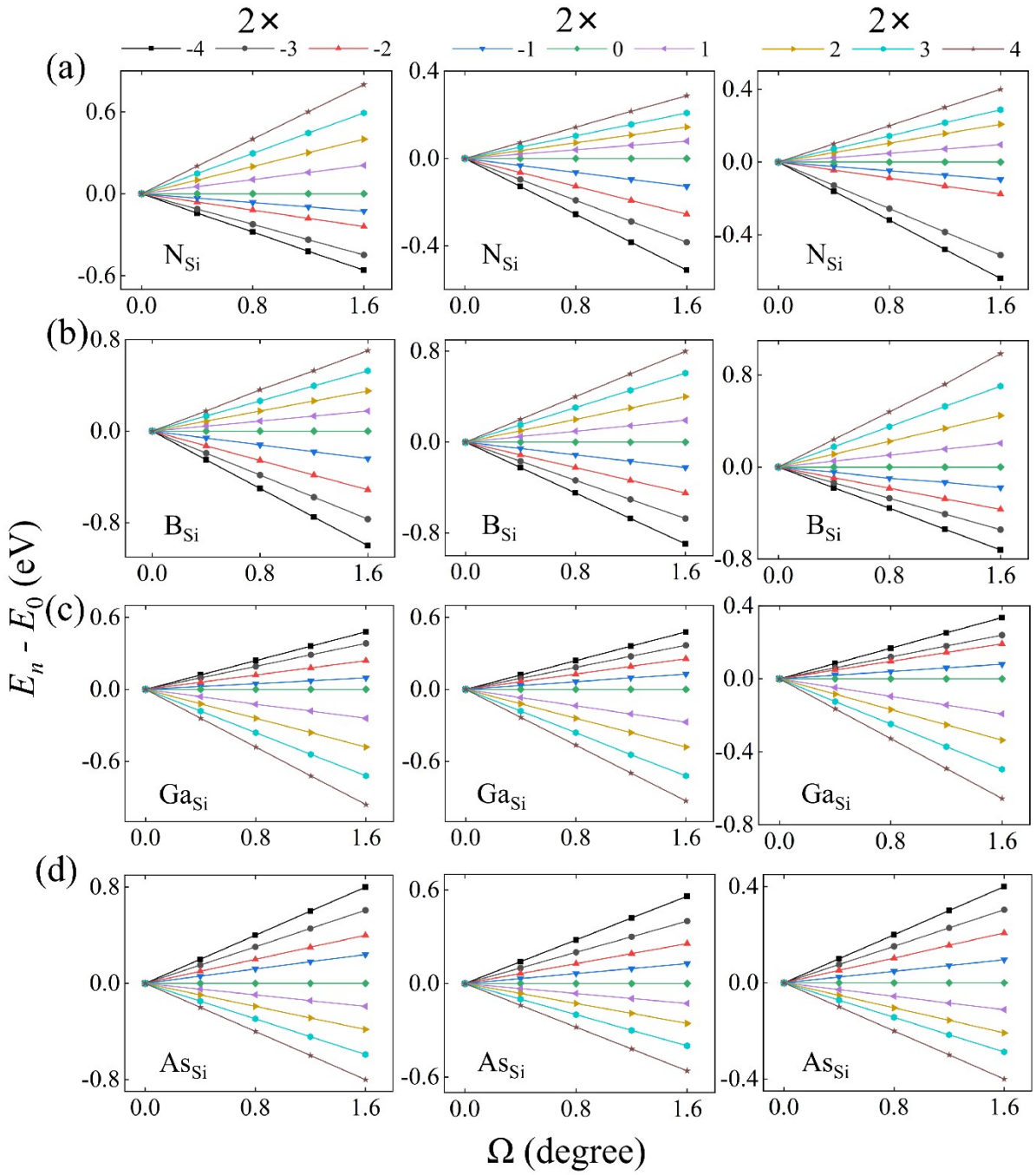

FIG. S5 The relative formation energy versus bending angle for [111]-oriented SiNWs with D = 4.43 nm in expanded supercells with doping at sites sites n = -4, -3, -2, -1, 0, 1, 2, 3, 4. The first, second, and third columns correspond to 2×, 3×, and 4× supercells, respectively, with (a) N doping, (b) B doping, (c) Ga doping, and (d) As doping.

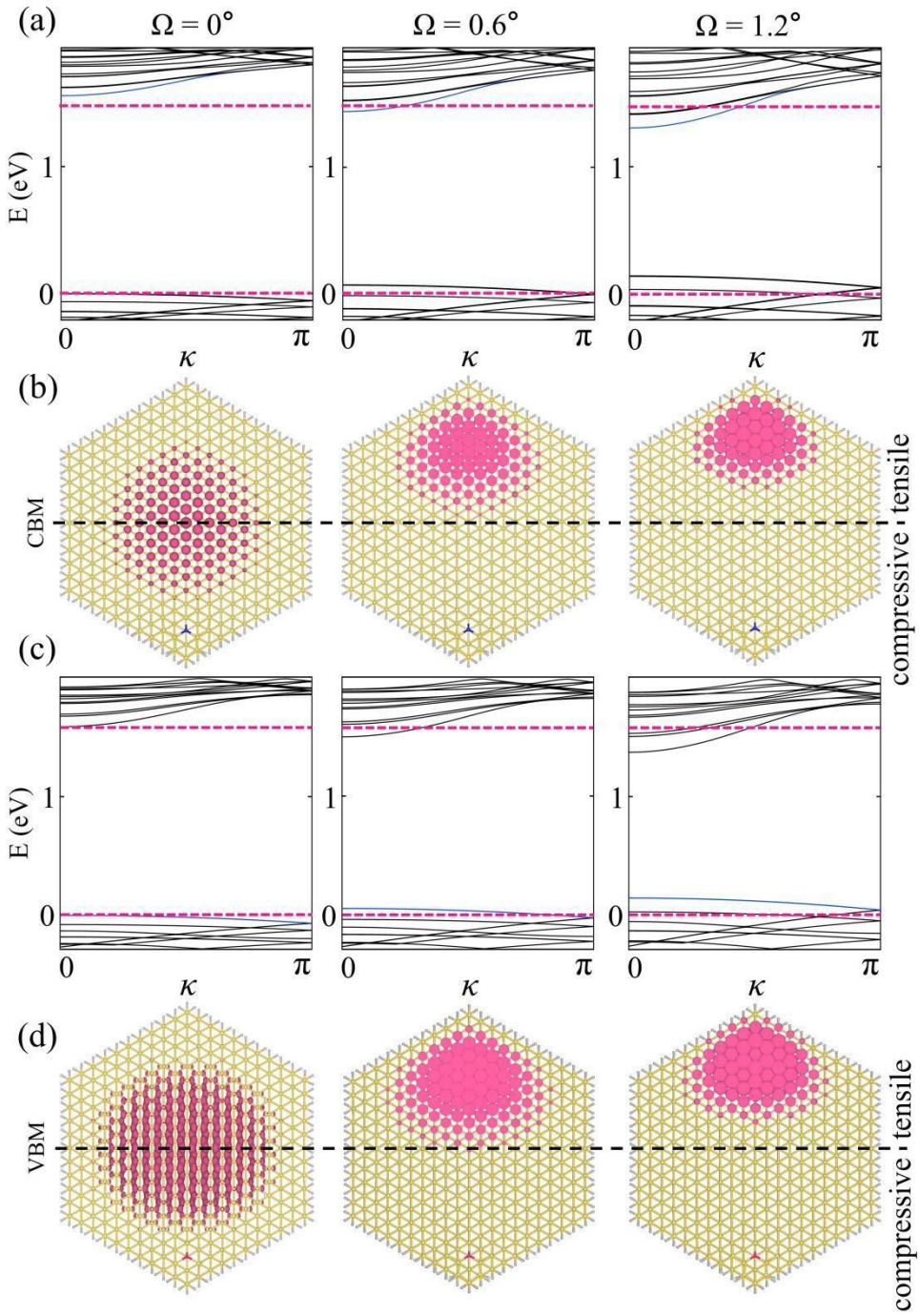

FIG. S6 [111]-oriented SiNW with a 2× expanded supercell and a diameter of ***D*** = 4.43 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.6°and Ω = 1.2°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72 × 10^{-6} e $Å^{-3}$.

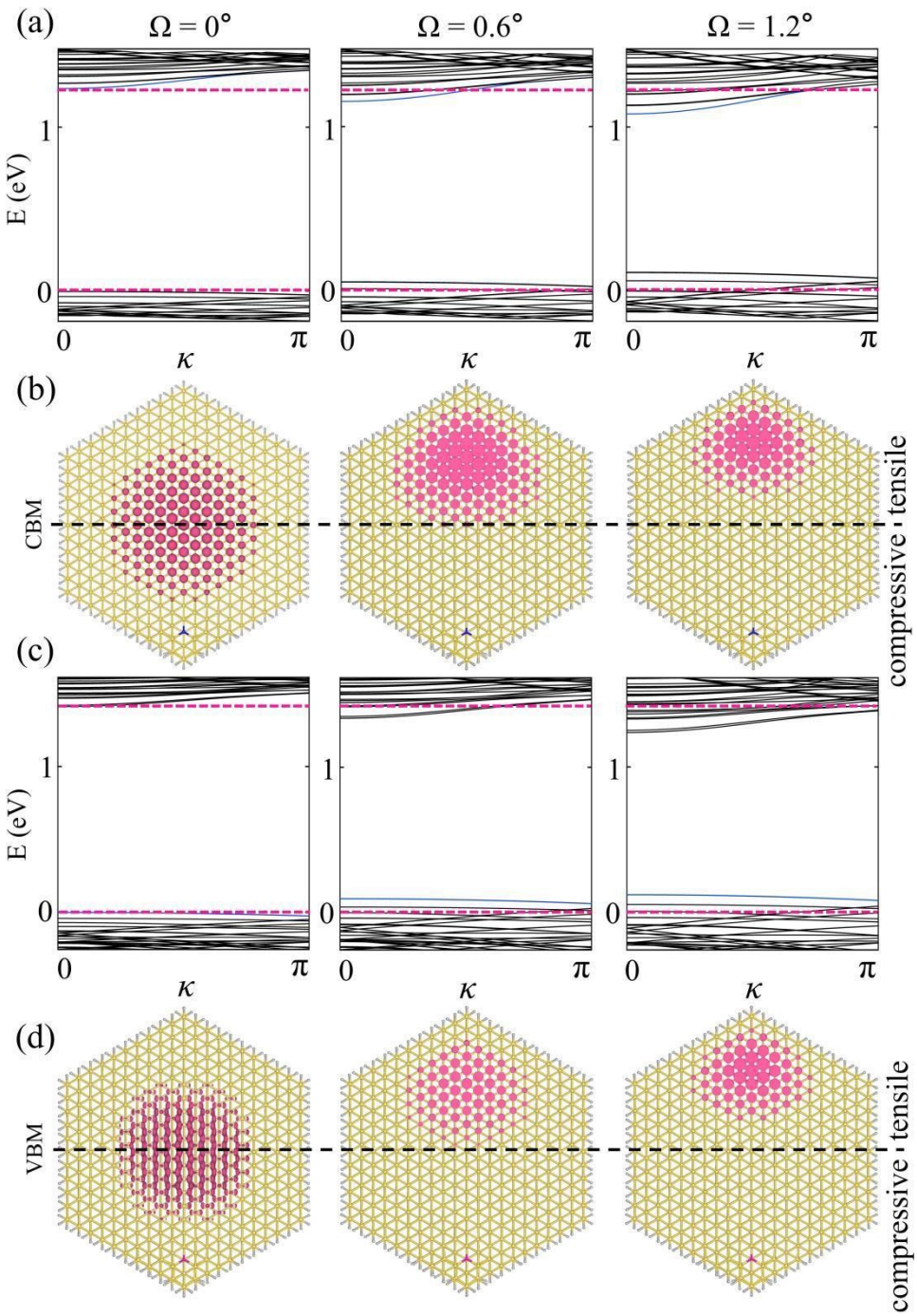

FIG. S7 [111]-oriented SiNW with a 3× expanded supercell and a diameter of ***D*** = 4.43 nm after (a) (b) N and (c) (d) B doped at position *n* = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.6°and Ω = 1.2°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72 × 10^{-6} e Å^{-3}.

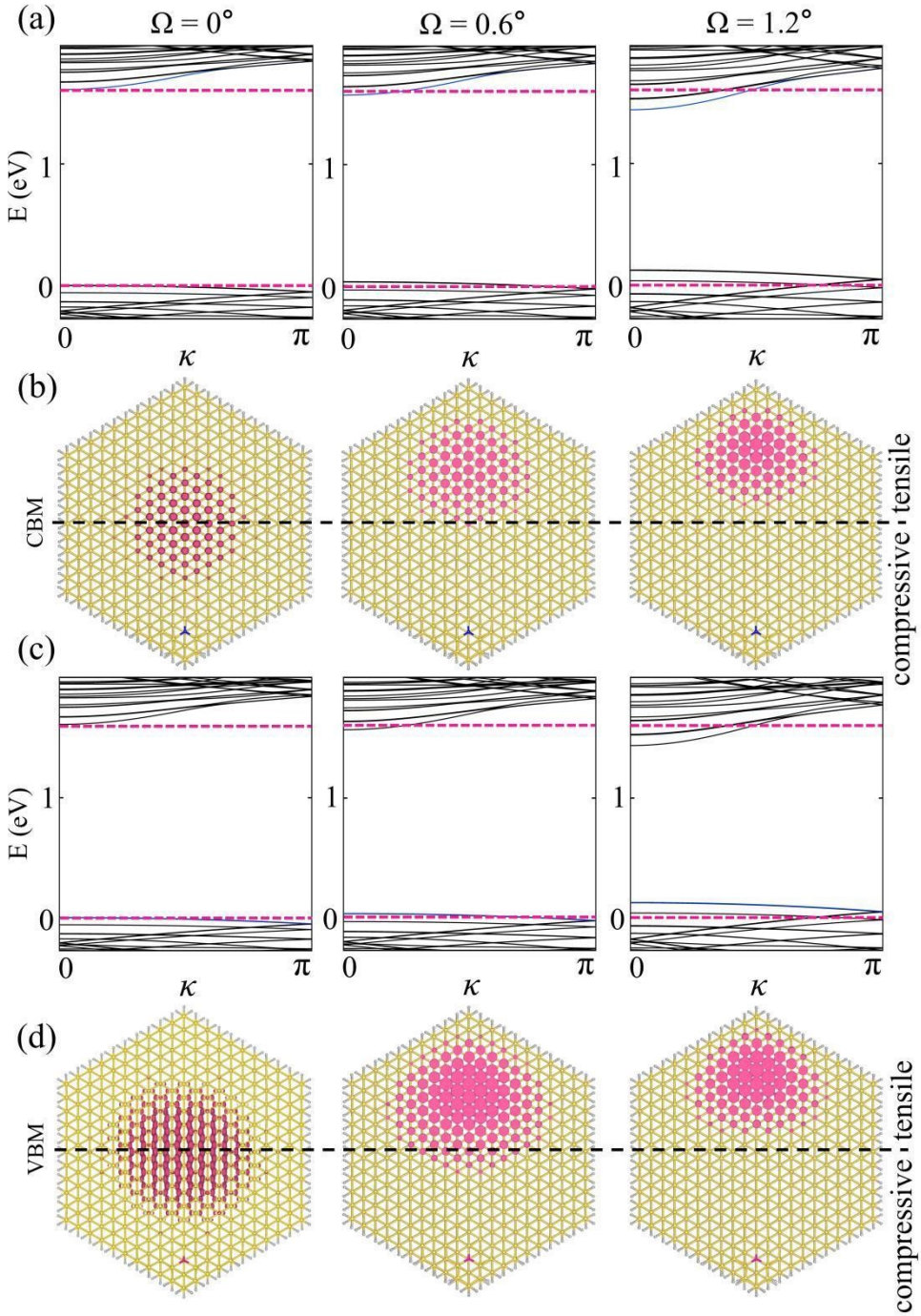

FIG. S8 [111]-oriented SiNW with a 4× expanded supercell and a diameter of ***D*** = 4.43 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.6°and Ω = 1.2°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72 × 10^{-6} e $Å^{-3}$.

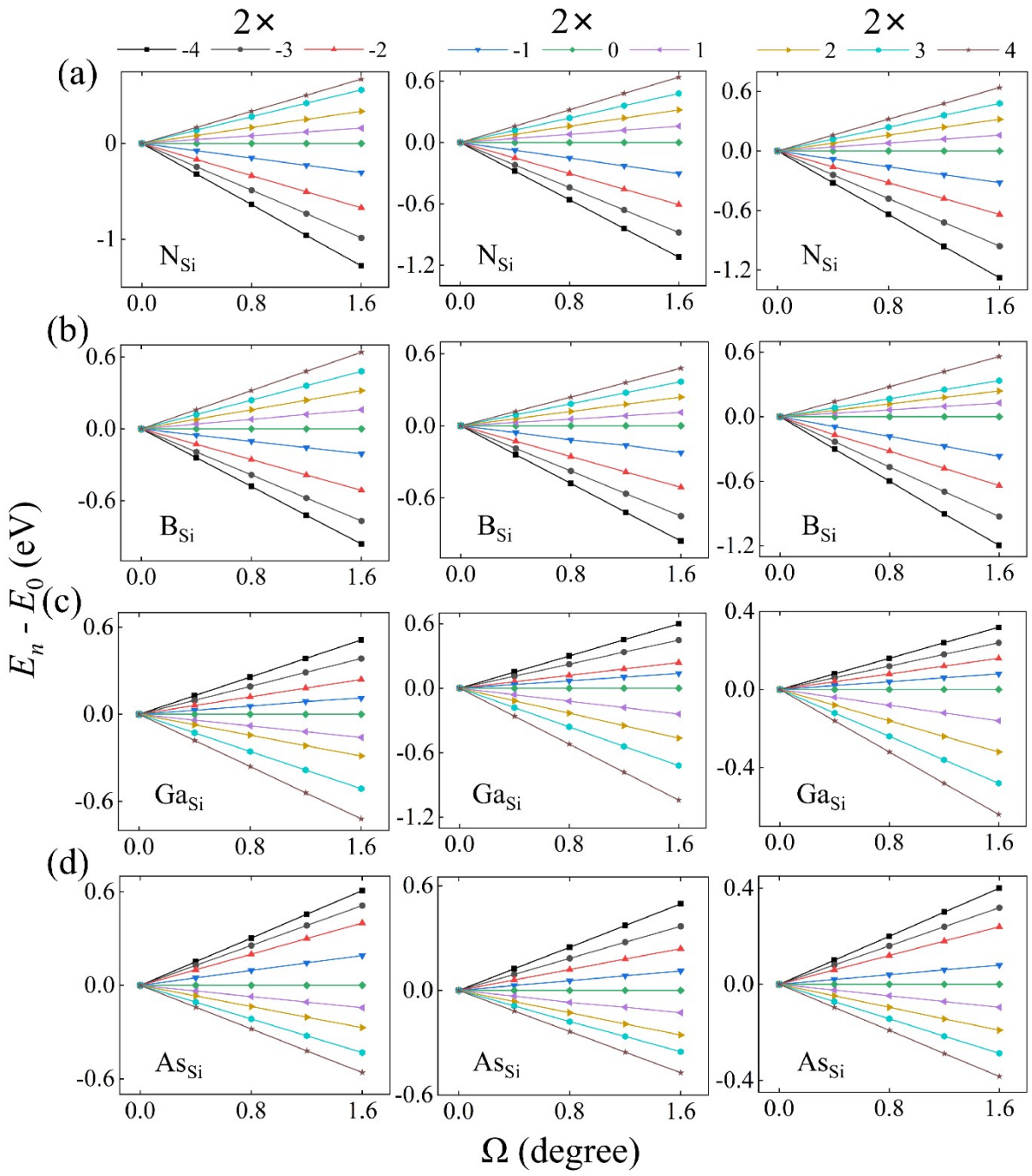

FIG. S9 The relative formation energy versus bending angle for [001]-oriented SiNWs with D = 4.22 nm in expanded supercells with doping at sites sites n = -4, -3, -2, -1, 0, 1, 2, 3, 4. The first, second, and third columns correspond to 2×, 3×, and 4× supercells, respectively, with (a) N doping, (b) B doping, (c) Ga doping, and (d) As doping.

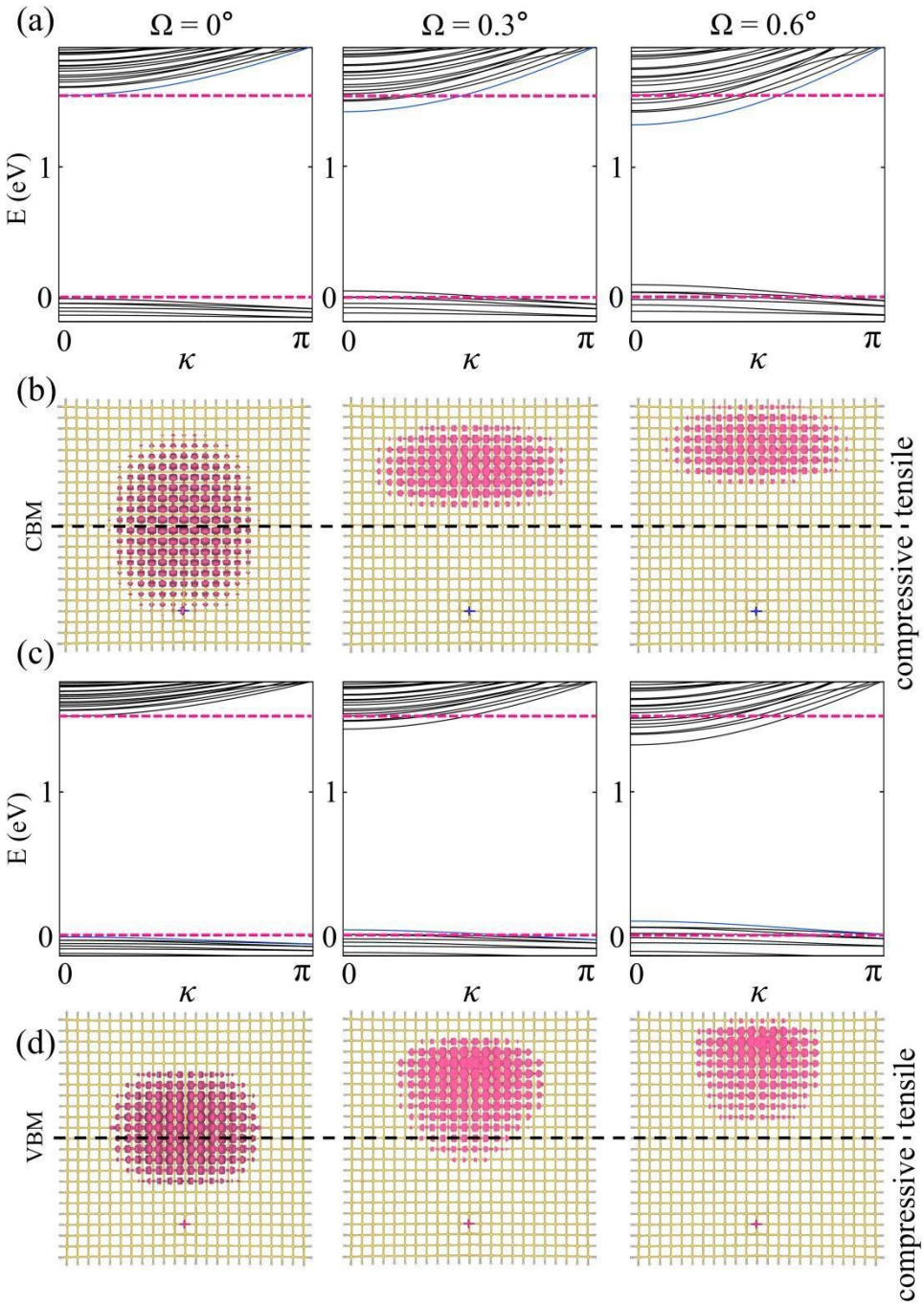

FIG. S10 [001]-oriented SiNW with a 2× expanded supercell and a diameter of ***D*** = 4.22 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3°and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72 × 10^{-6} e $Å^{-3}$.

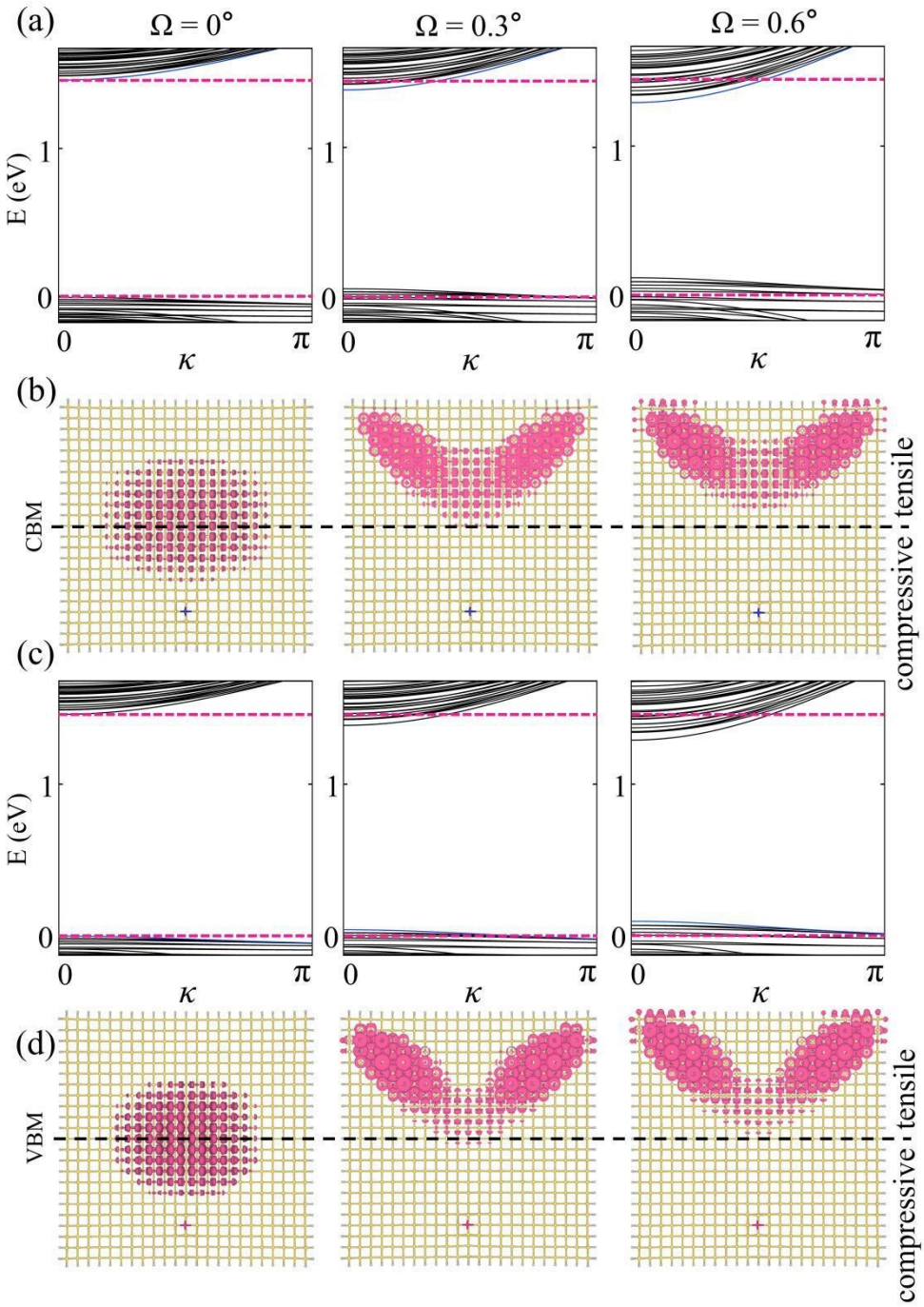

FIG. S11 [001]-oriented SiNW with a 3× expanded supercell and a diameter of ***D*** = 4.22 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3°and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72 × 10^{-6} e Å^{-3}.

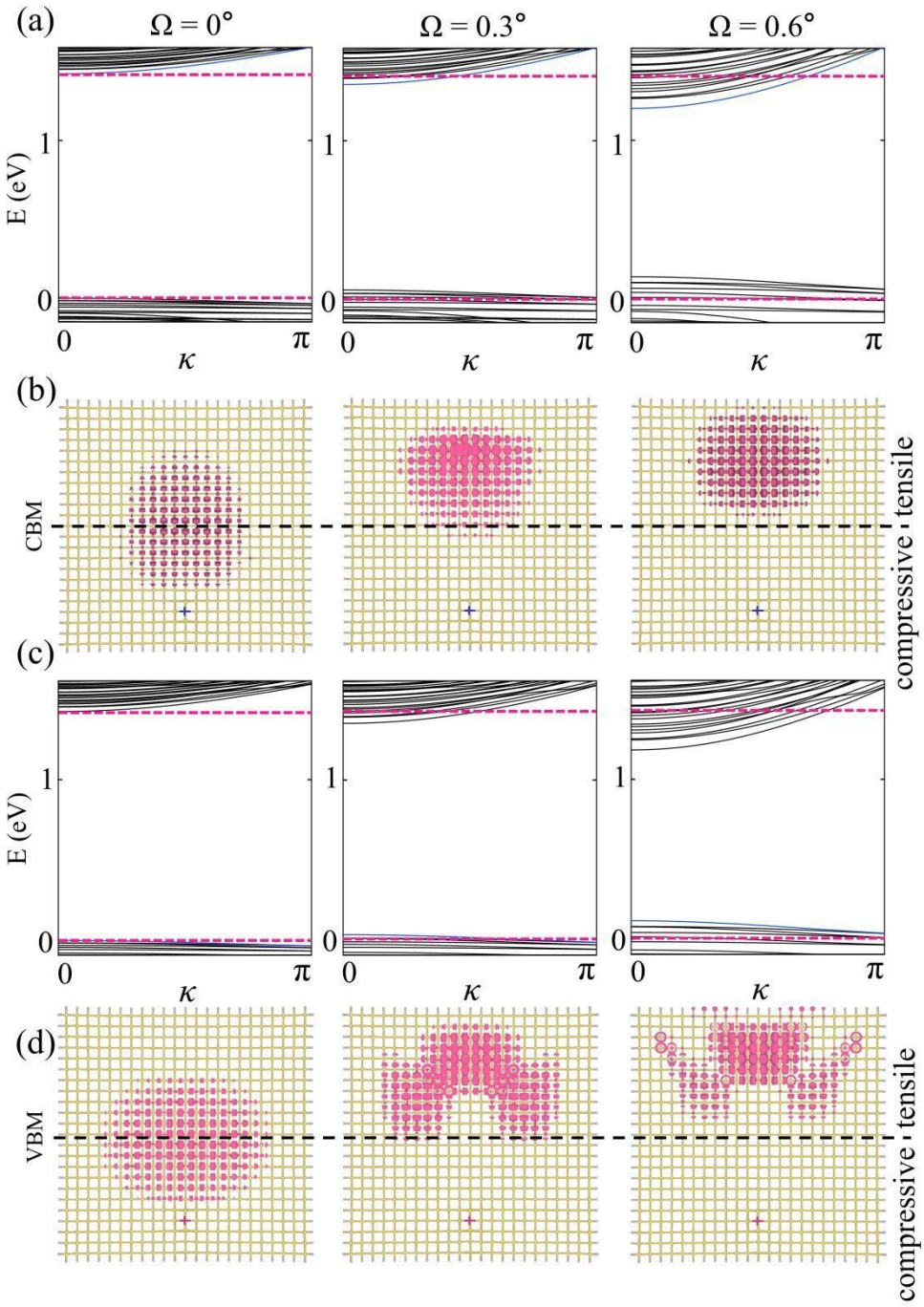

FIG. S12 [001]-oriented SiNW with a 4× expanded supercell and a diameter of ***D*** = 4.22 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3°and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72 × 10^{-6} e Å^{-3}.

S5. Calculations with different diameters.

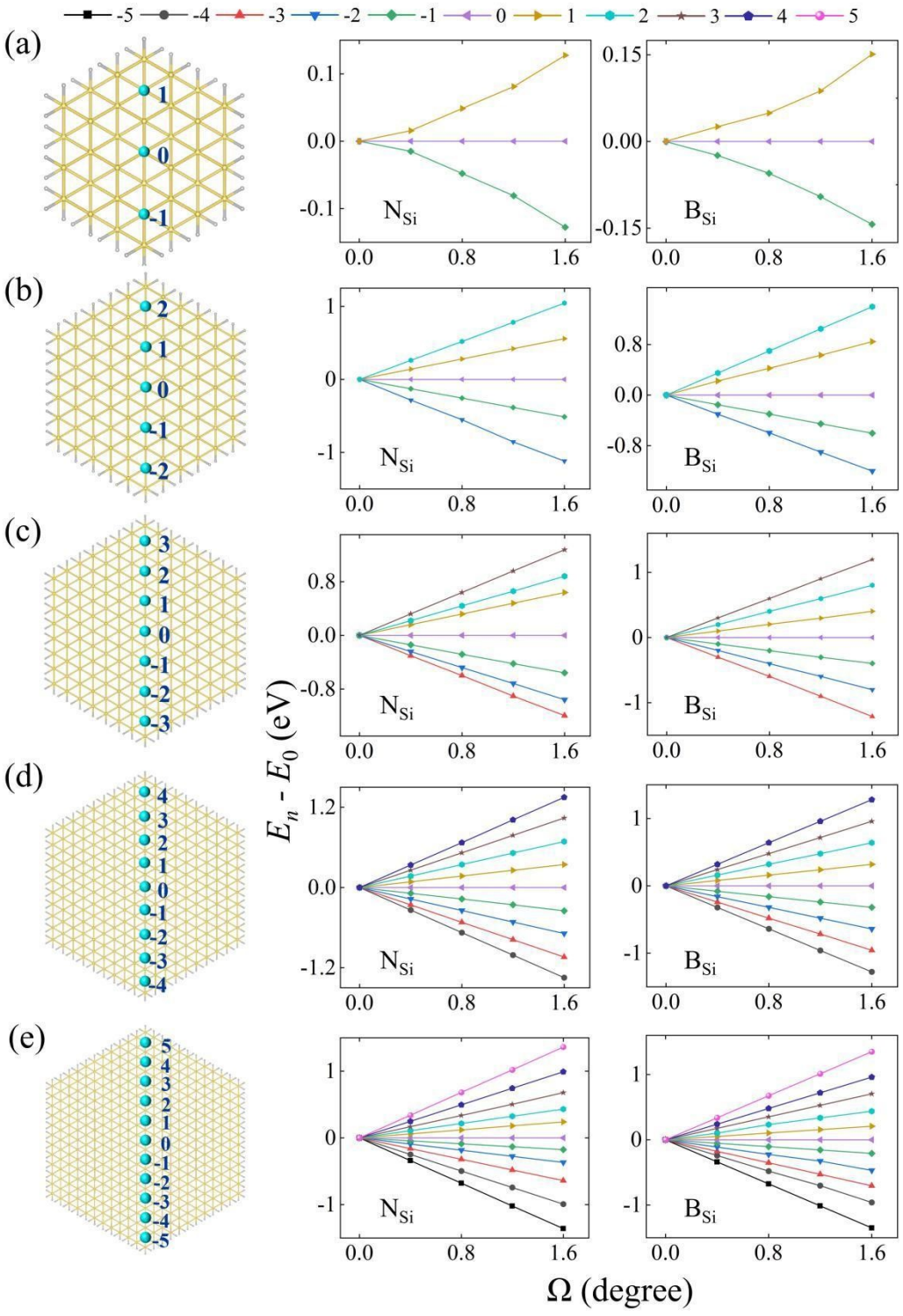

FIG. S13 [111]-oriented SiNW with a diameter of ***D*** = (a) 1.32 nm, (b) 2.24 nm, (c) 3.1 nm, (d) 3.99 nm, (e) 4.89 nm, with 11 doping sites (blue balls): sites n = 1, 2, 3, 4, 5 are on the tensile side, sites n = -1, -2, -3, -4, -5 are on the compressive side, and site n = 0 is on the neutral

surface. The last two columns are The relative formation energy $E_n - E_0$ at site n versus bending angle Ω for various doping cases, denoted as X_{Si} (X = B, N), where the host Si atom is substituted with the dopant X atom.

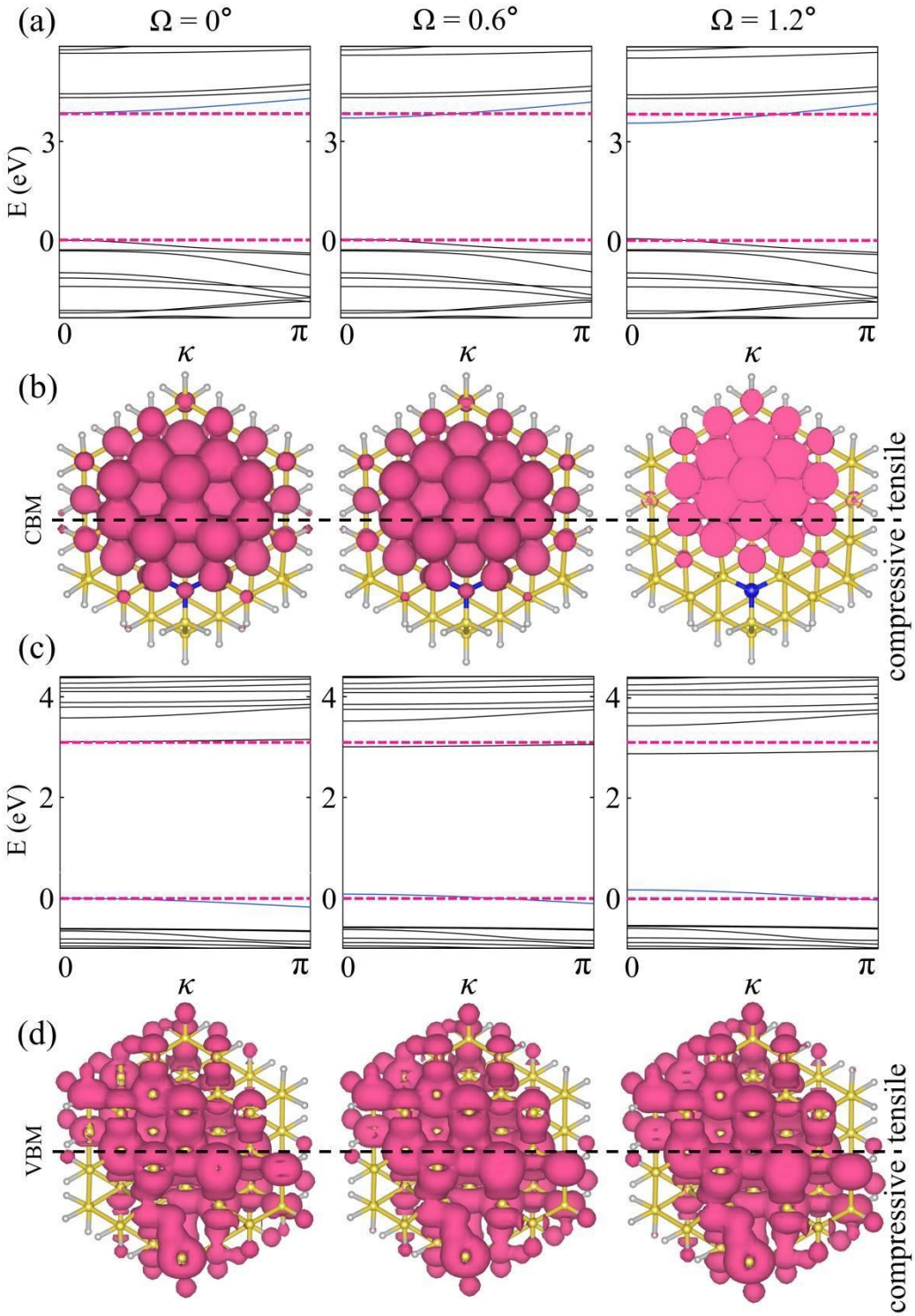

FIG. S14 [111]-oriented SiNW with a diameter of $\boldsymbol{D}$ = 1.32 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with $\Omega = 0.6°$ and $\Omega = 1.2°$. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72×10^{-6} e Å^{-3}.

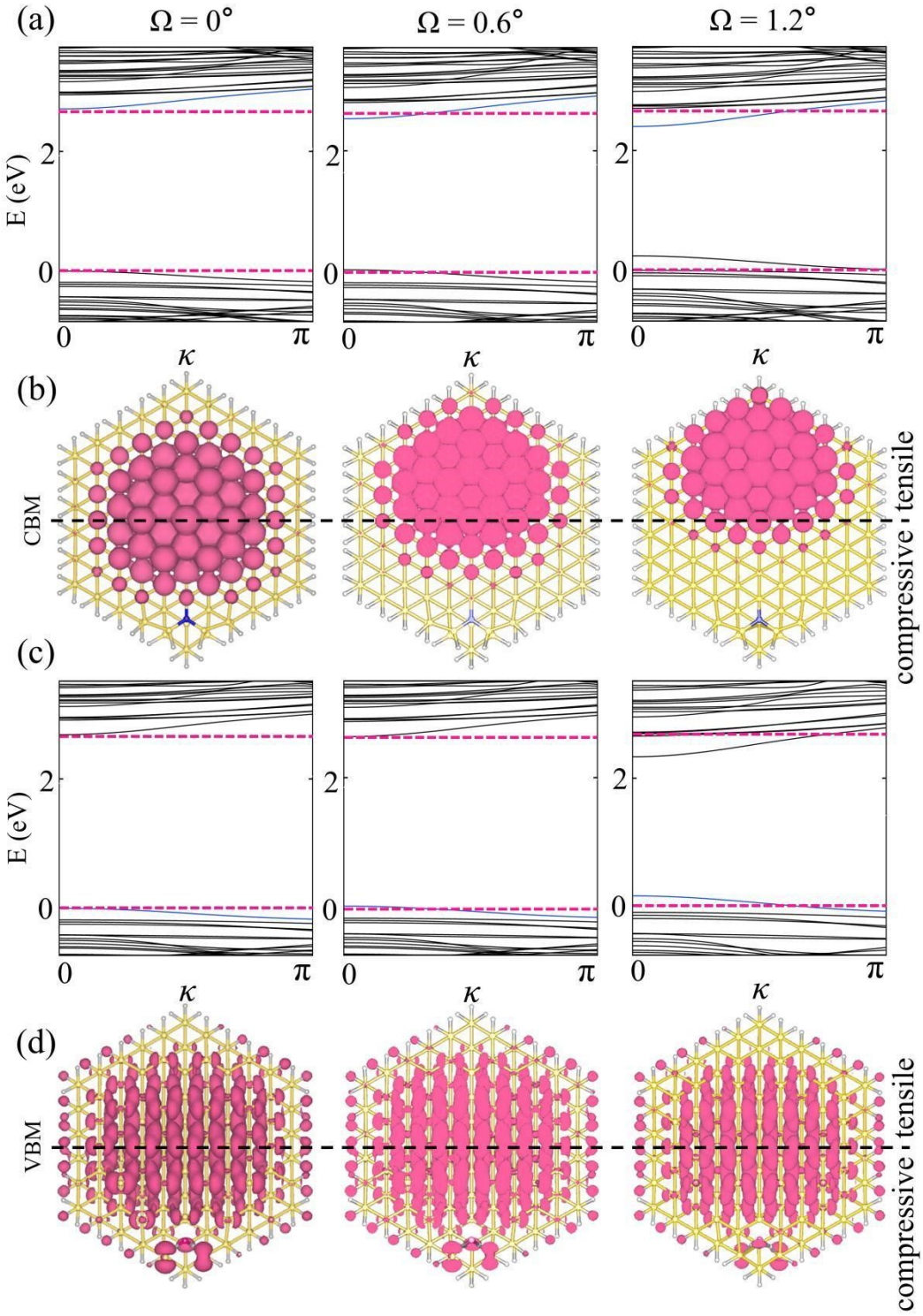

FIG. S15 [111]-oriented SiNW with a diameter of ***D*** = 2.24 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.6° and Ω = 1.2°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72×10^{-6} e Å^{-3}.

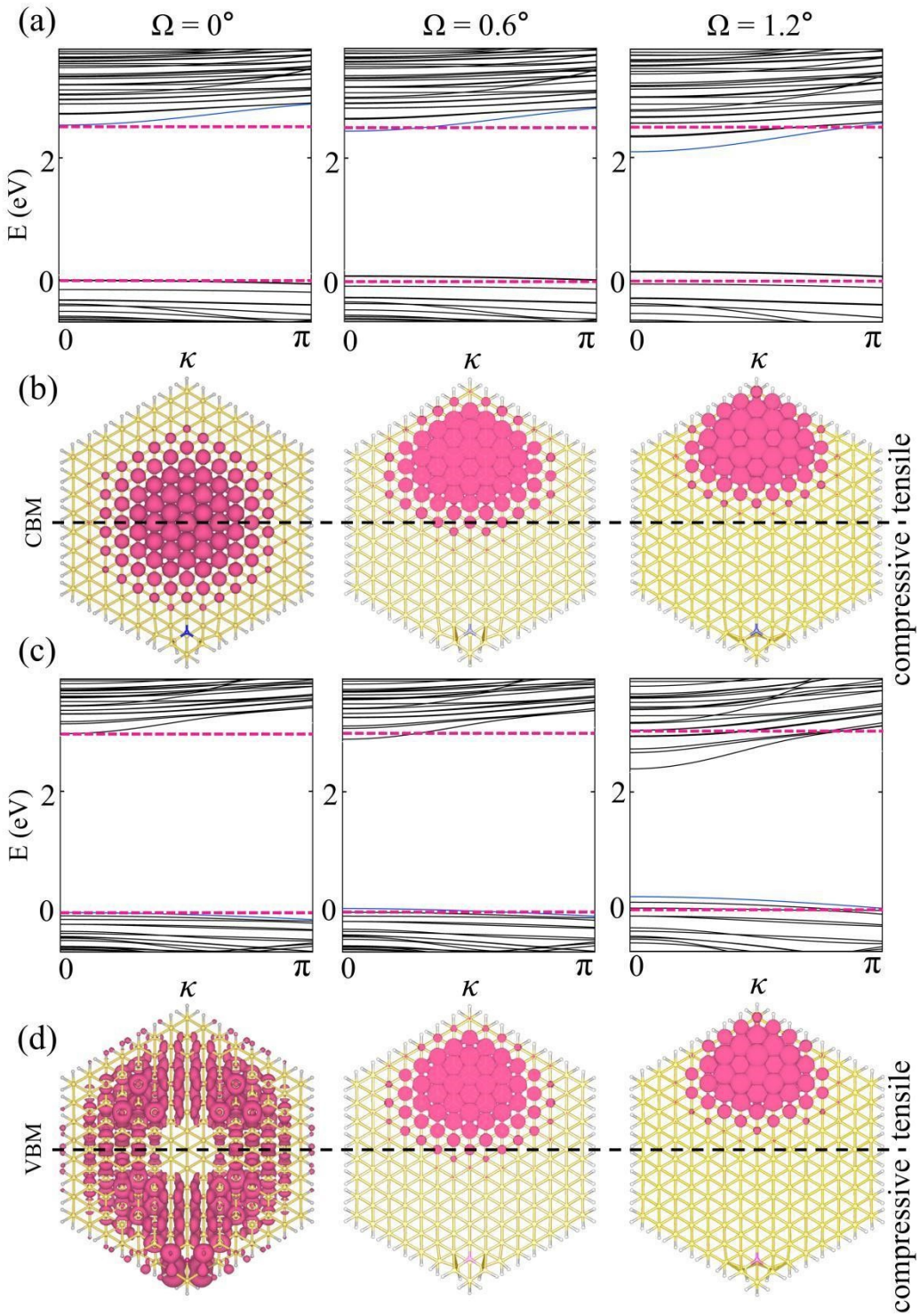

FIG. S16 [111]-oriented SiNW with a diameter of ***D*** = 3.1 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.6° and Ω = 1.2°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72×10^{-6} e Å^{-3}.

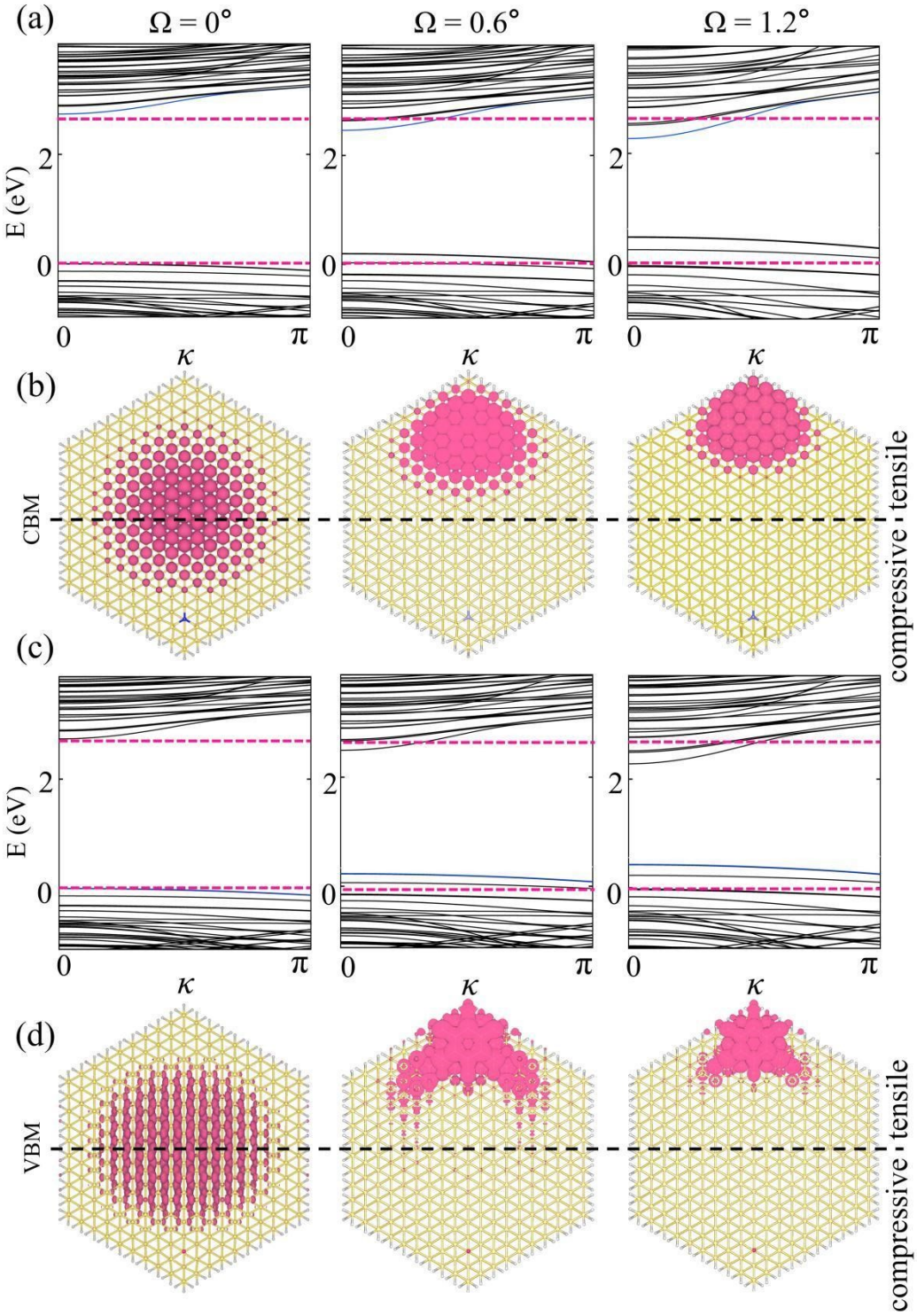

FIG. S17 [111]-oriented SiNW with a diameter of ***D*** = 3.99 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles

with Ω = 0.6° and Ω = 1.2°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72 × 10^{-6} e $Å^{-3}$.

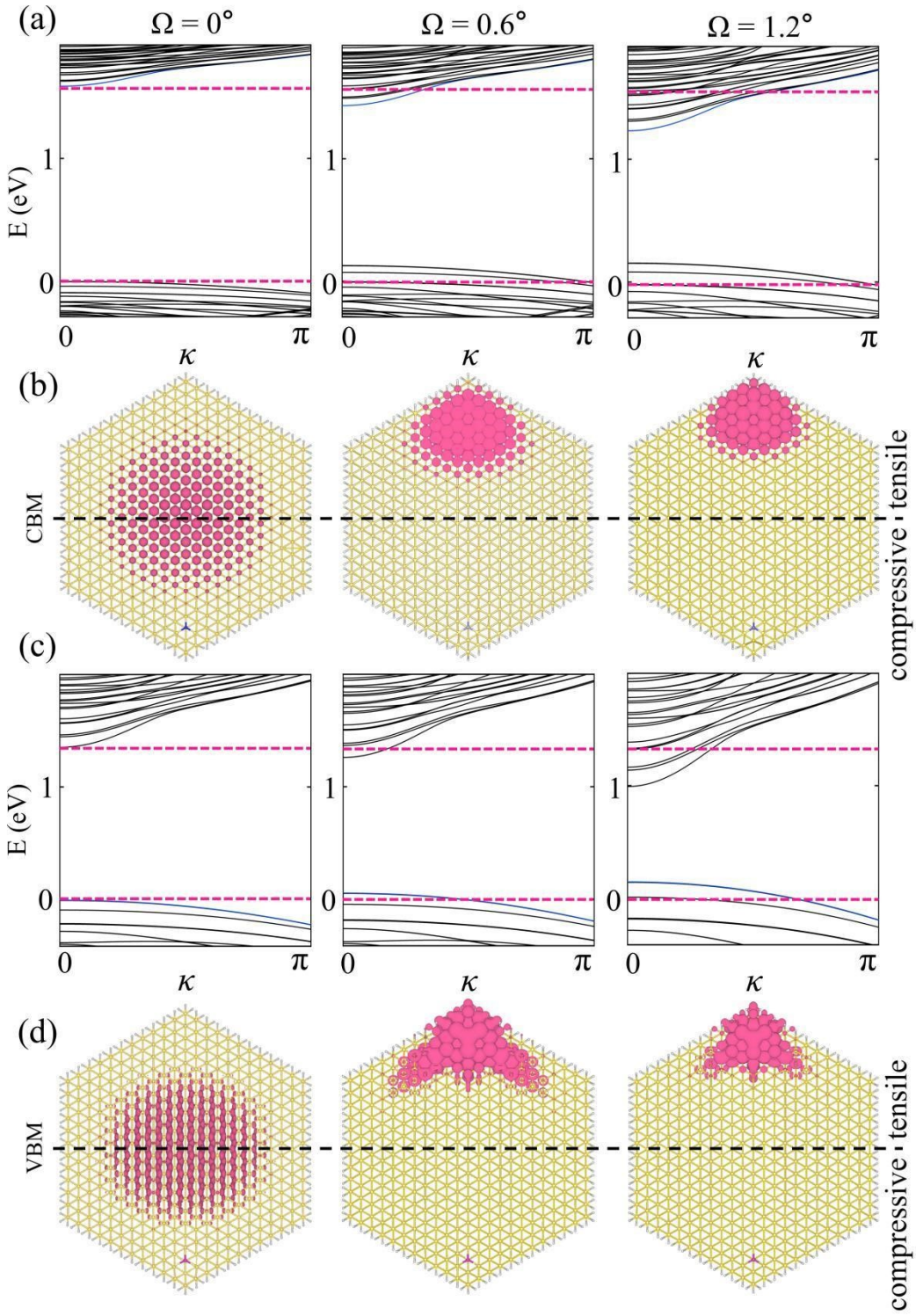

FIG. S18 [111]-oriented SiNW with a diameter of ***D*** = 4.89 nm after (a) (b) N and (c) (d) B doped at position *n* = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles

with Ω = 0.6° and Ω = 1.2°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72 × 10^{-6} e $Å^{-3}$.

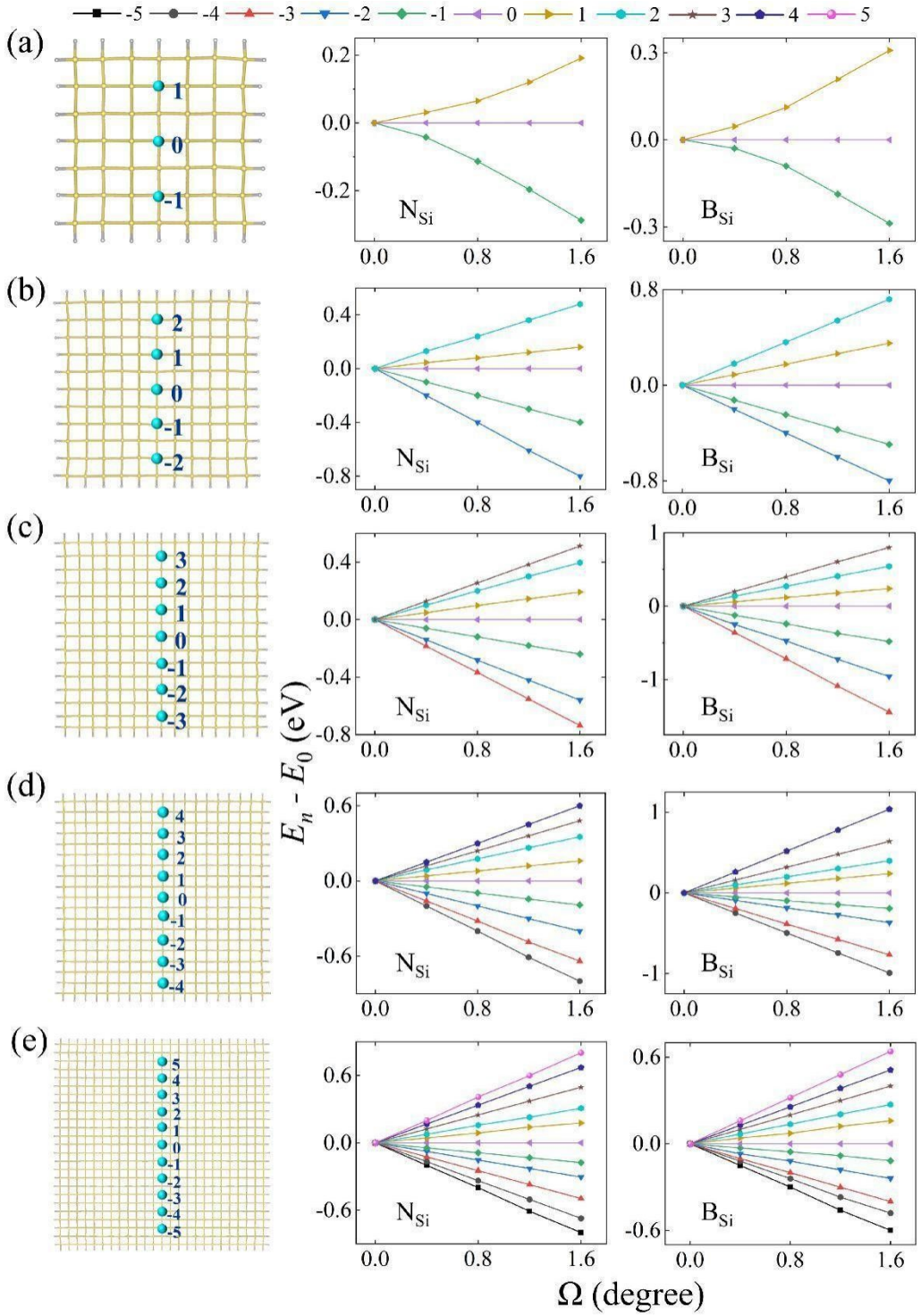

FIG. S19 [001]-oriented SiNW with a diameter of ***D*** = (a) 1.15 nm, (b) 1.92 nm, (c) 2.68 nm, (d) 3.45 nm, (e) 4.61 nm, with 11 doping sites (blue balls): sites *n* = 1, 2, 3, 4, 5 are on the

tensile side, sites n = -1, -2, -3, -4, -5 are on the compressive side, and site n = 0 is on the neutral surface. The last two columns are The relative formation energy $E_n - E_0$ at site n versus bending angle Ω for various doping cases, denoted as X_{Si} (X = B, N), where the host Si atom is substituted with the dopant X atom.

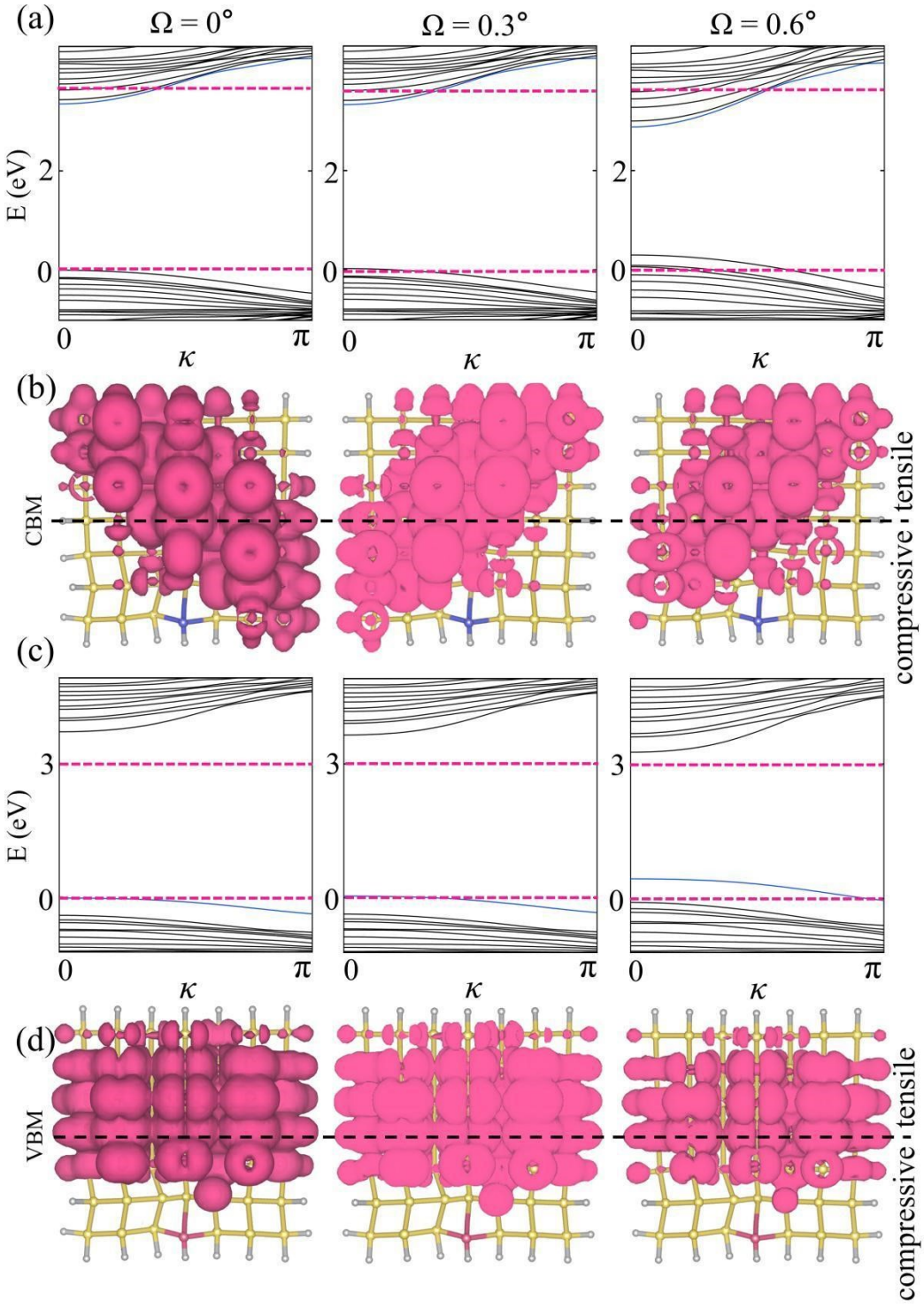

FIG. S20 [001]-oriented SiNW with a diameter of ***D*** = 1.15 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3° and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72×10^{-6} e Å^{-3}.

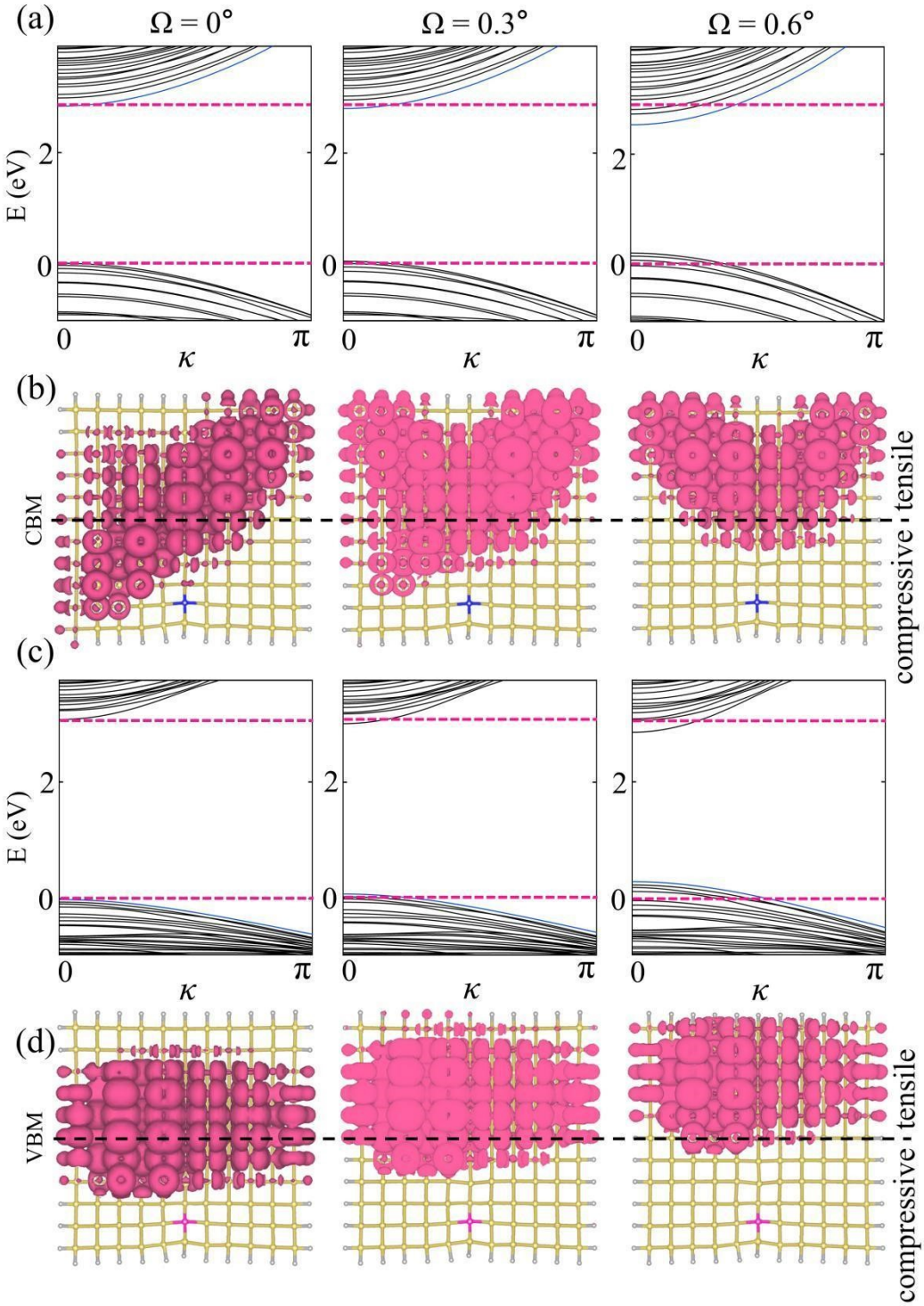

FIG. S21 [001]-oriented SiNW with a diameter of ***D*** = 1.92 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3° and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72×10^{-6} e Å^{-3}.

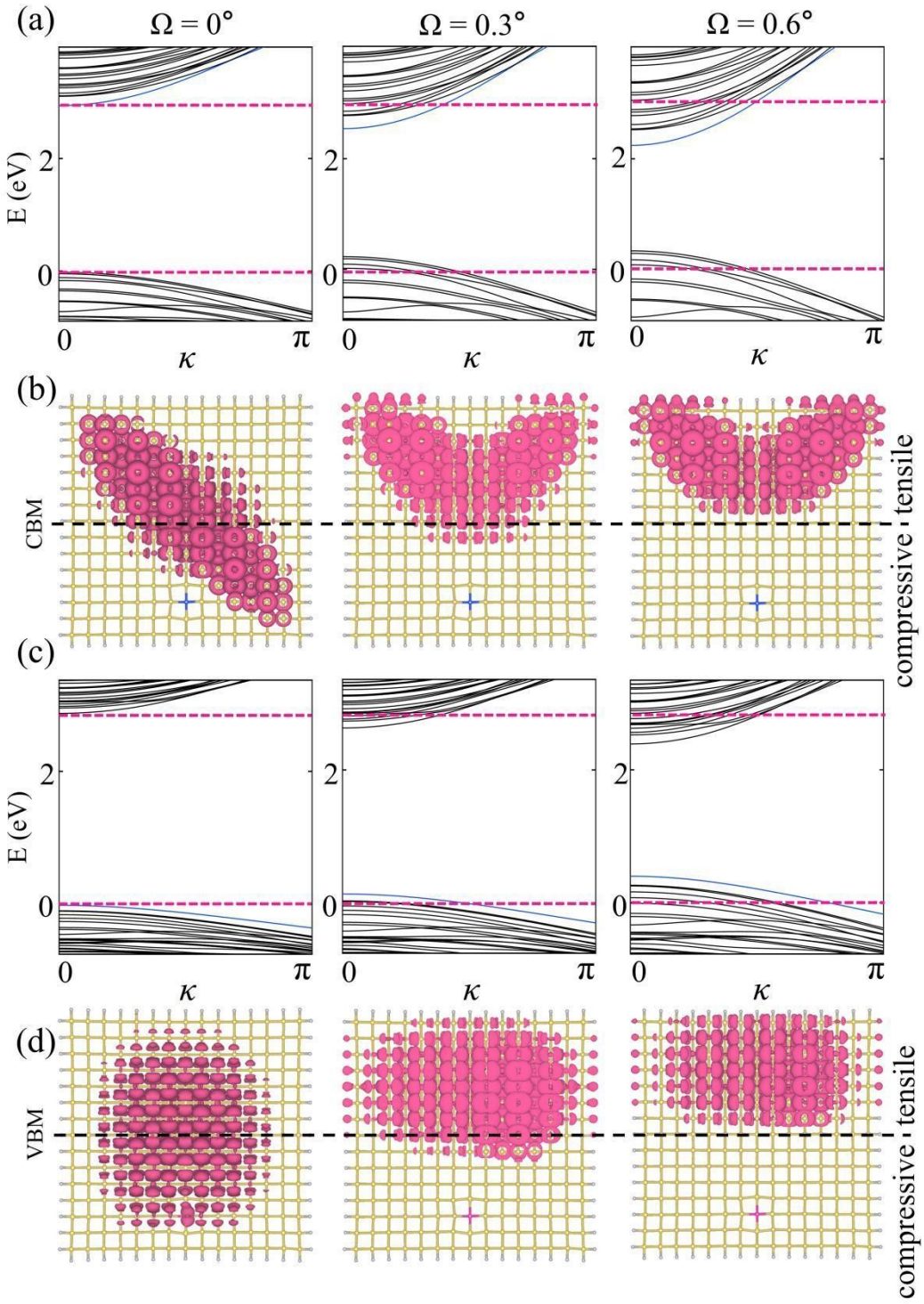

FIG. S22 [001]-oriented SiNW with a diameter of ***D*** = 2.68 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3° and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72×10^{-6} e Å^{-3}.

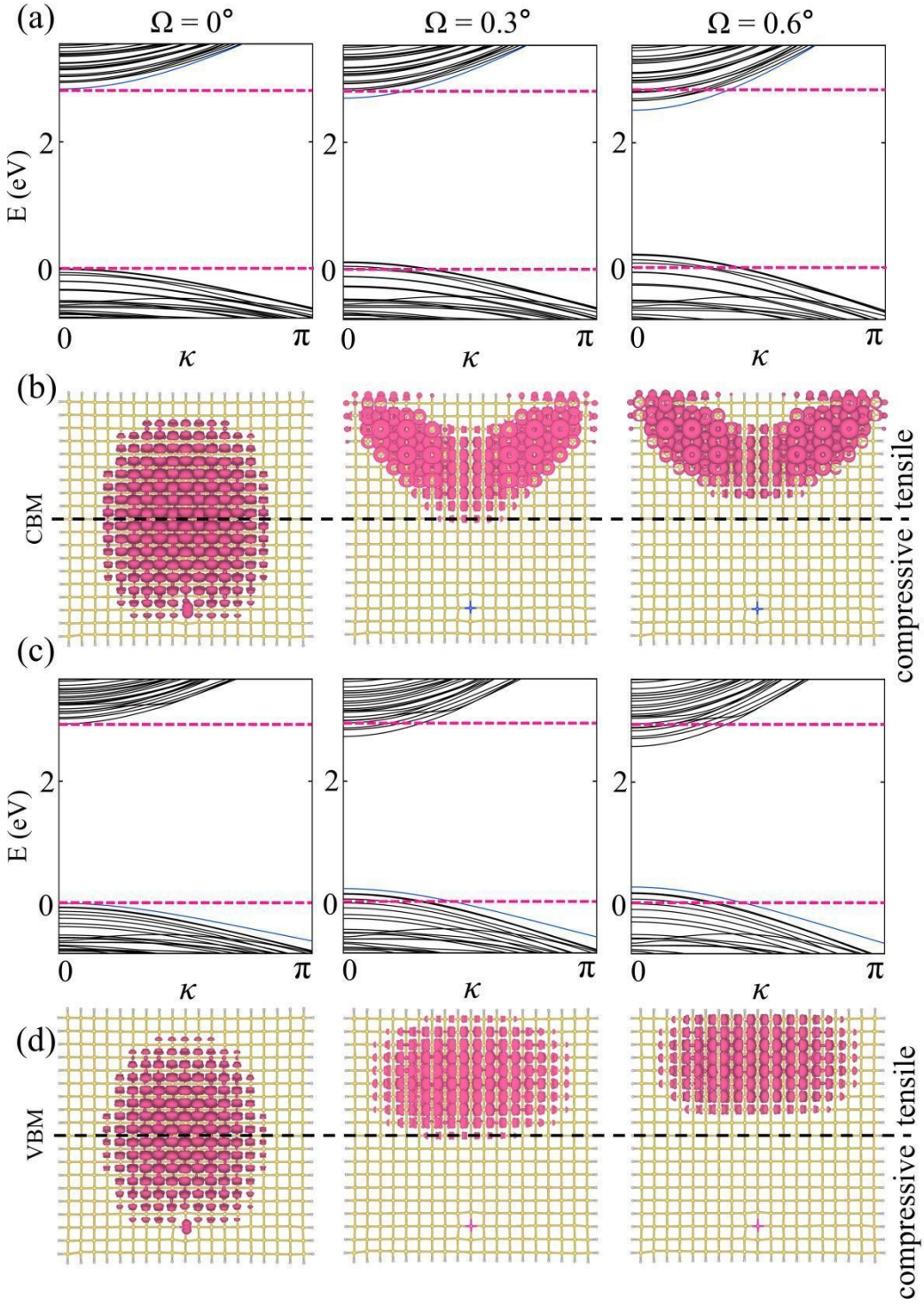

FIG. S23 [001]-oriented SiNW with a diameter of ***D*** = 3.45 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3° and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72×10^{-6} e Å^{-3}.

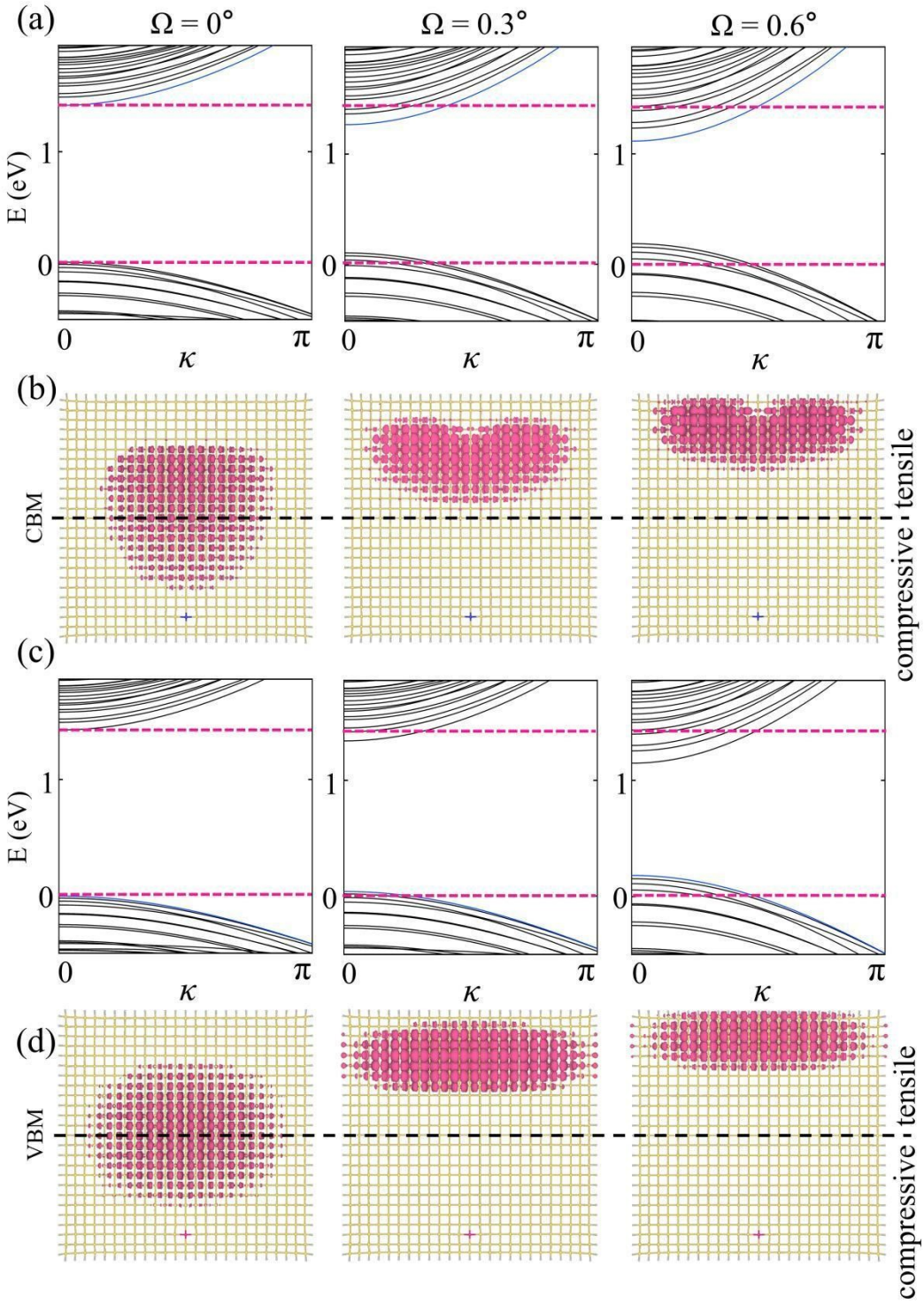

FIG. S24 [001]-oriented SiNW with a diameter of ***D*** = 4.61 nm after (a) (b) N and (c) (d) B doped at position n = -4. (a) (c) Electronic energy bands for strain-free NW and bending angles with Ω = 0.3° and Ω = 0.6°. Electronic density distribution (pink spheres) for the (b) CBM state and (d) the VBM state. The isosurface level is 1.72×10^{-6} e Å^{-3}.