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

Supporting Information

General Existences of Flexural Mode Doublets in Nanowires Targeting Vectorial Sensing Applications

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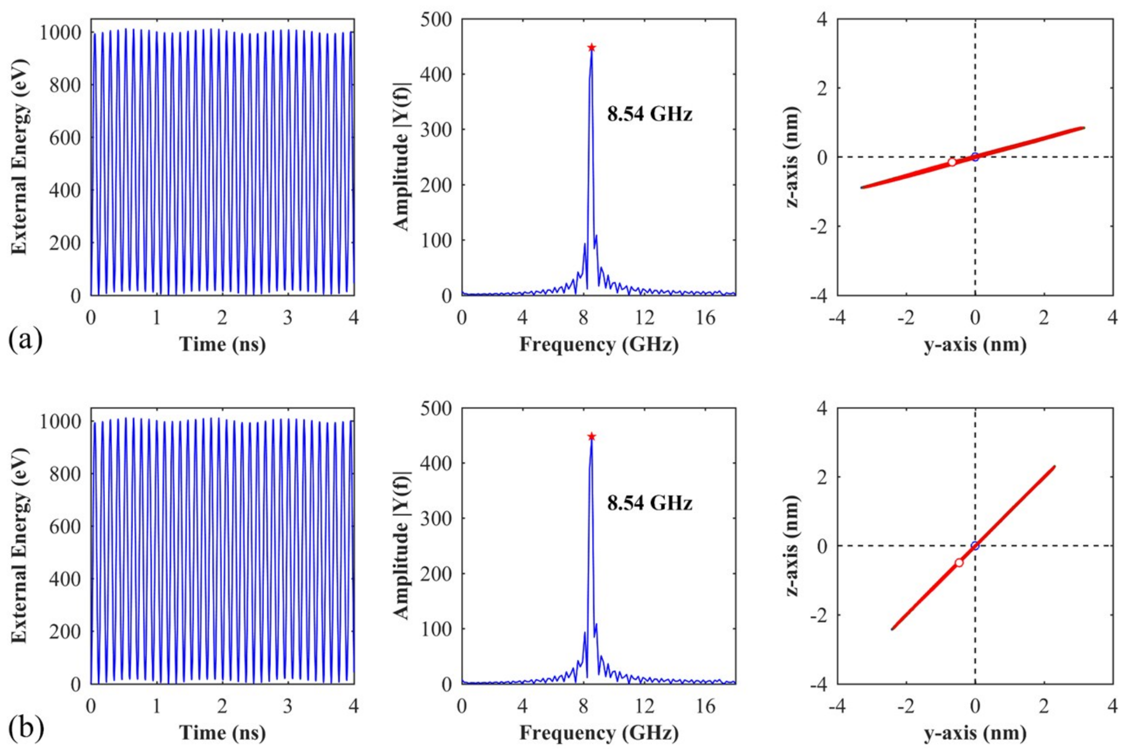
S1. Vibrational behaviors of <111> Cu NWs

The vibrational properties of <111> Cu NWs under different excitation angles, including 15°, 45°, and 75°. As compared in **Figure S1**, a single natural frequency is resolved for all three cases and the trajectory of the center of mass is well confined along the excitation direction. These observations signify a single flexural mode for the <111> Cu NW.



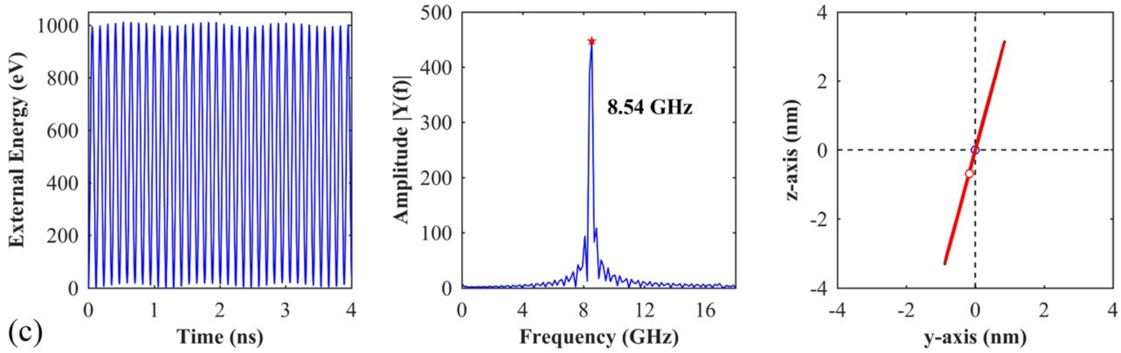
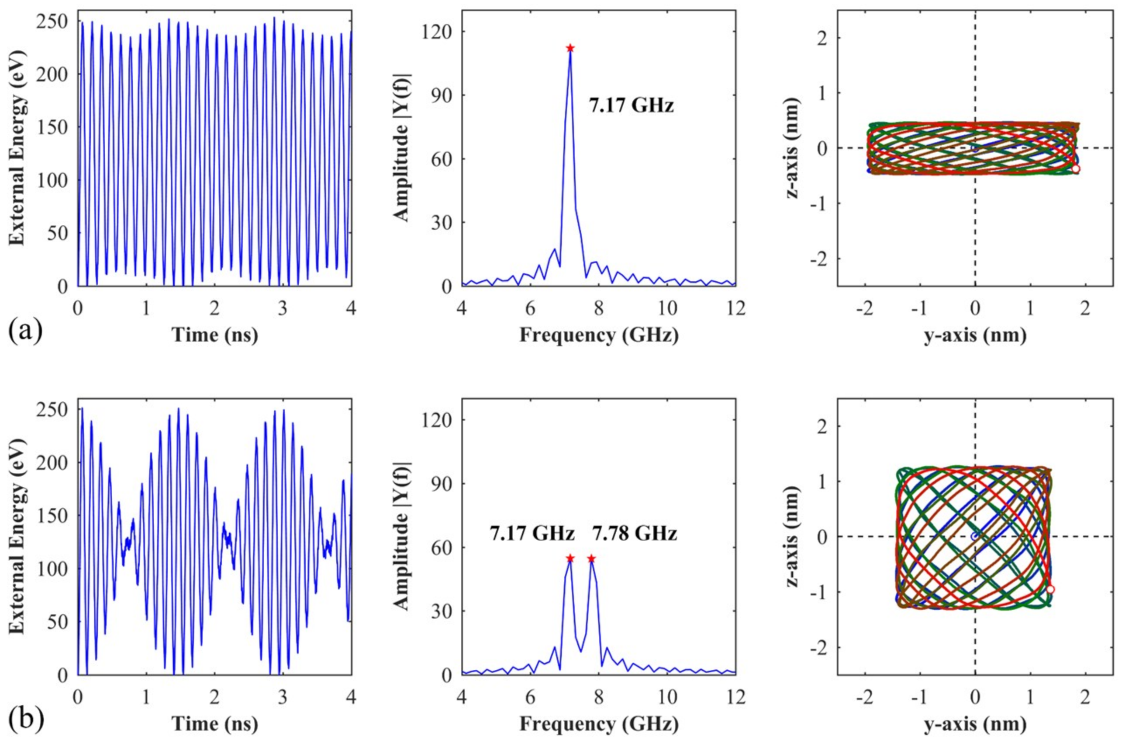


Figure S1. Vibrational behaviors of <111> orientated Cu NW. The time history of the external energy (left panel), the corresponding frequency spectrum obtained from FFT analysis (middle panel), and the trajectory of the center of mass (right panel) for the NW under the excitation with an angle of: (a) 15°, (b) 45°, and (c) 75° with its orthogonal $[1\bar{2}1]$ direction.

S2. Vibrational behaviors of <110> Cu NWs

The vibrational properties of <110> Cu NWs under different excitation angles, including 15°, 45°, and 75°. As compared in **Figure S2**, the trajectory of the center of mass is not following the excitation direction, which exhibits a two-dimensional movement, which indicating that the <110> Cu NW is under a dual mode vibration. However, it is noticed that such information is not obvious from the time history of the external energy or the frequency spectrum due to the relatively large vibration amplitude in one of the orthogonal directions.



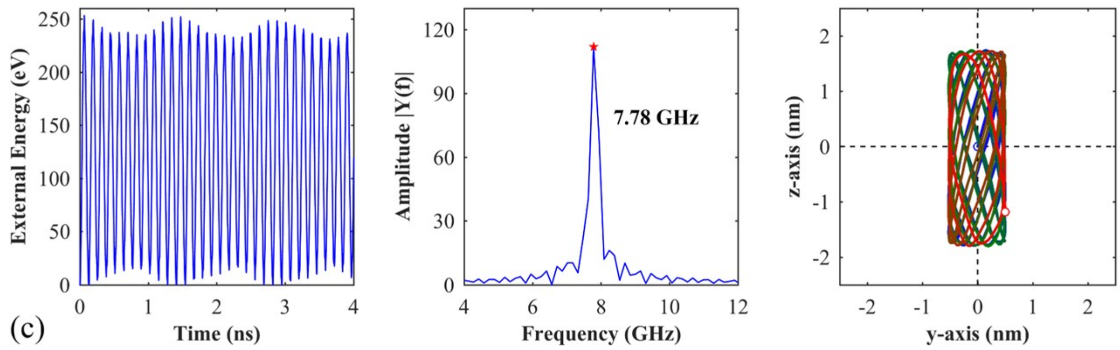


Figure S2. Vibrational behaviors of <110> orientated Cu NW. The time history of the external energy (left panel), the corresponding frequency spectrum obtained from FFT analysis (middle panel), and the trajectory of the center of mass (right panel) for the NW under the excitation with an angle of: (a) 15°, (b) 45°, and (c) 75° with its orthogonal [$\bar{1}$10] direction.

S3. Frequency spectrum for the <110> Cu NWs with different slenderness ratio

As shown in **Figure S3**, with increasing slenderness, it is harder to distinguish the two resonance frequencies from the frequency spectrum. In order to resolve both natural frequencies, a much longer simulation is expected.

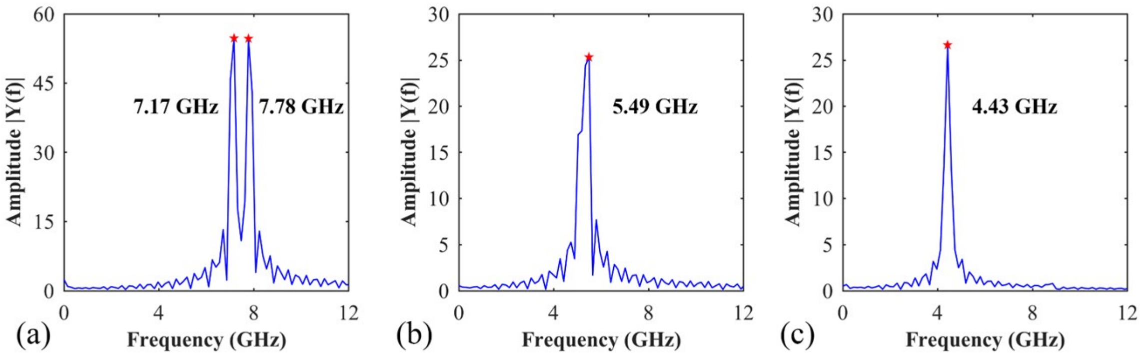


Figure S3. The resonance frequency of the <110> orientated Cu NW. The frequency spectrum obtained from FFT analysis for the NW with a slenderness ratio of: (a) 8.3; (b) 12.5; and (c) 16.7. Actuation has an angle of 45° with its orthogonal [$\bar{1}$10] direction.

S4. Vibrational behaviors of <112> and <100> Cu NWs

Comparison of the vibrational behaviors of <112> and <100> Cu NWs. As shown in **Figure S4**a, due to its directional dependent shear modulus, the <112> NW exhibits a dual mode vibration. In comparison, the <100> shows a single mode vibration with the trajectory of the center of mass following well with the excitation angle.

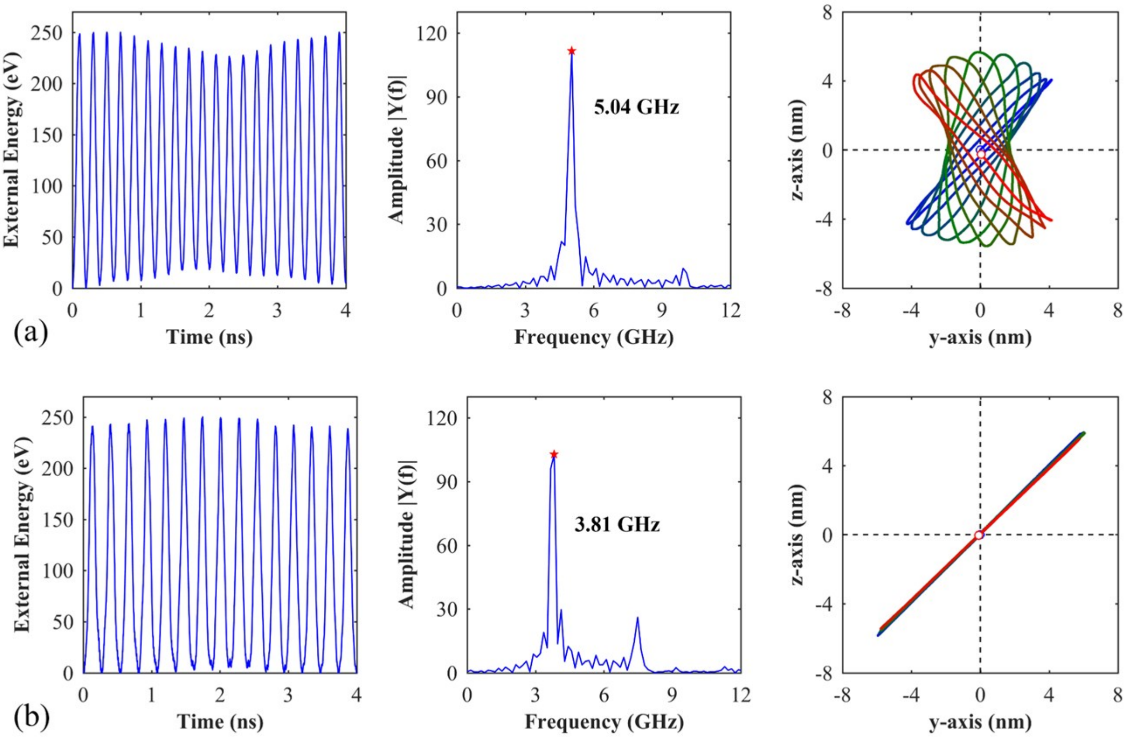
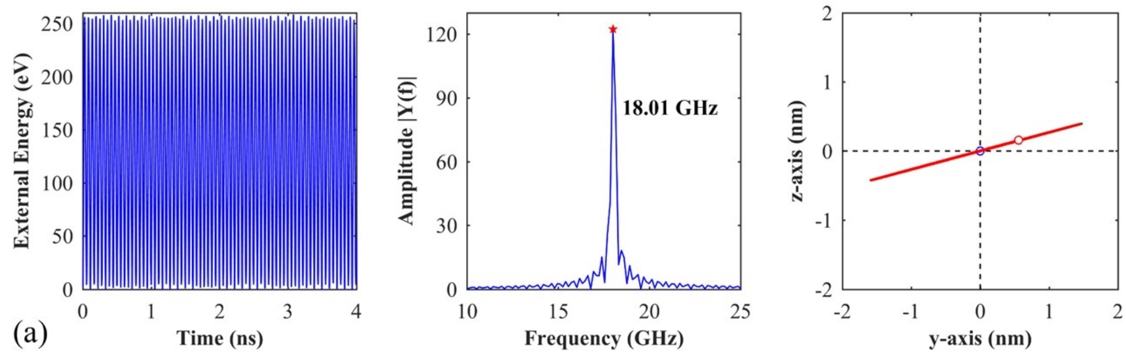


Figure S4. Vibrational behaviors of Cu NWs. The time history of the external energy (left panel), the corresponding frequency spectrum obtained from FFT analysis (middle panel), and the trajectory of the center of mass (right panel) for the: (a) <112> NW; and (b) <100> NW. Actuation has an angle of 45° with its orthogonal direction.

S5. Vibrational behaviors of <111> and <110> Si NWs

As shown in **Figure S5**a, the <111> Si NW always exhibit a single mode vibration while varying the excitation angle. The obtained natural frequencies are the same and the trajectory of the center of mass always adhere to the excitation directions. These results signify the single flexural mode in <111> Si NWs.



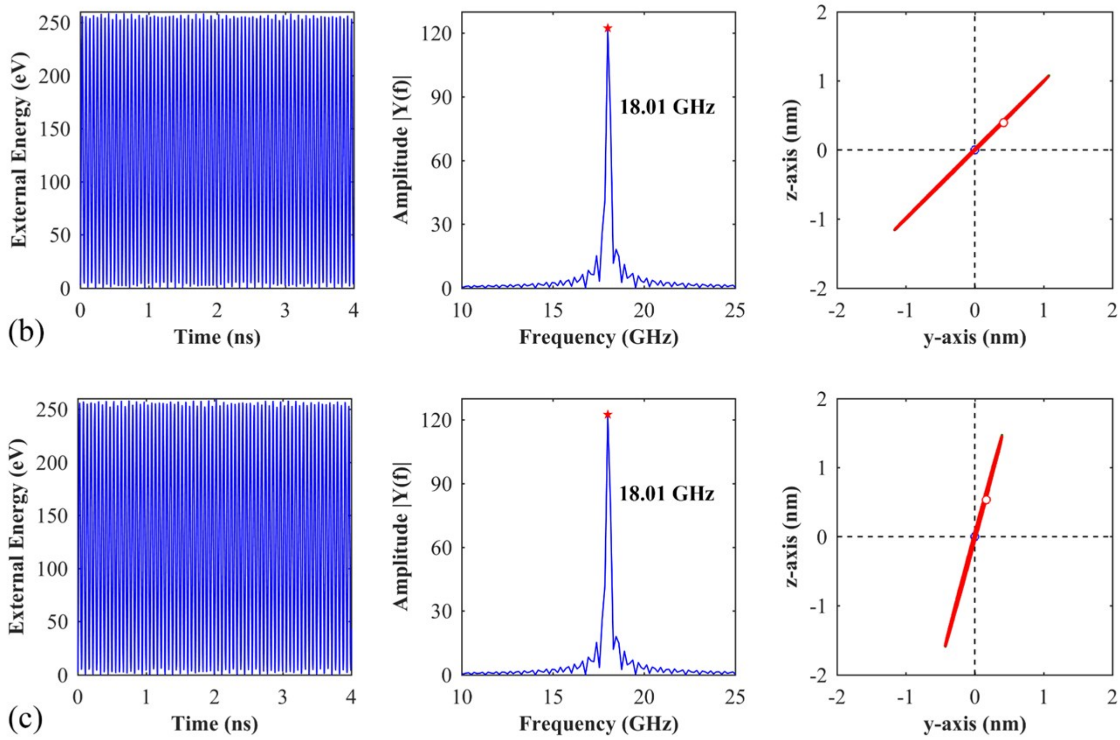
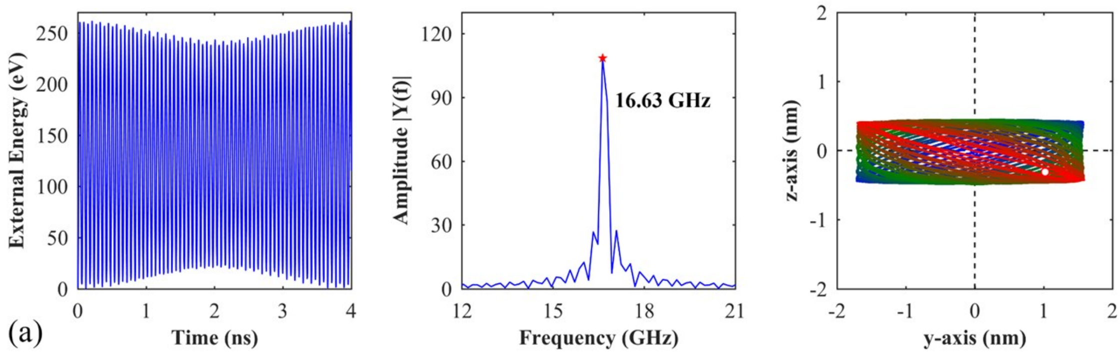


Figure S5. Vibrational behaviors of <111> orientated Si NW. The time history of the external energy (left panel), the corresponding frequency spectrum obtained from FFT analysis (middle panel), and the trajectory of the center of mass (right panel) for the NW under the excitation with an angle of: (a) 15°, (b) 45°, and (c) 75° with its orthogonal $[1\overline{2}1]$ direction.

In the other hand, the <110> Si NW shows a different vibration behavior while changing the excitation angle. Specifically, two natural frequencies are detected and the trajectories of the center of mass always exhibit a two-dimensional movement. These results signify the dual flexural mode in <110> Si NWs.



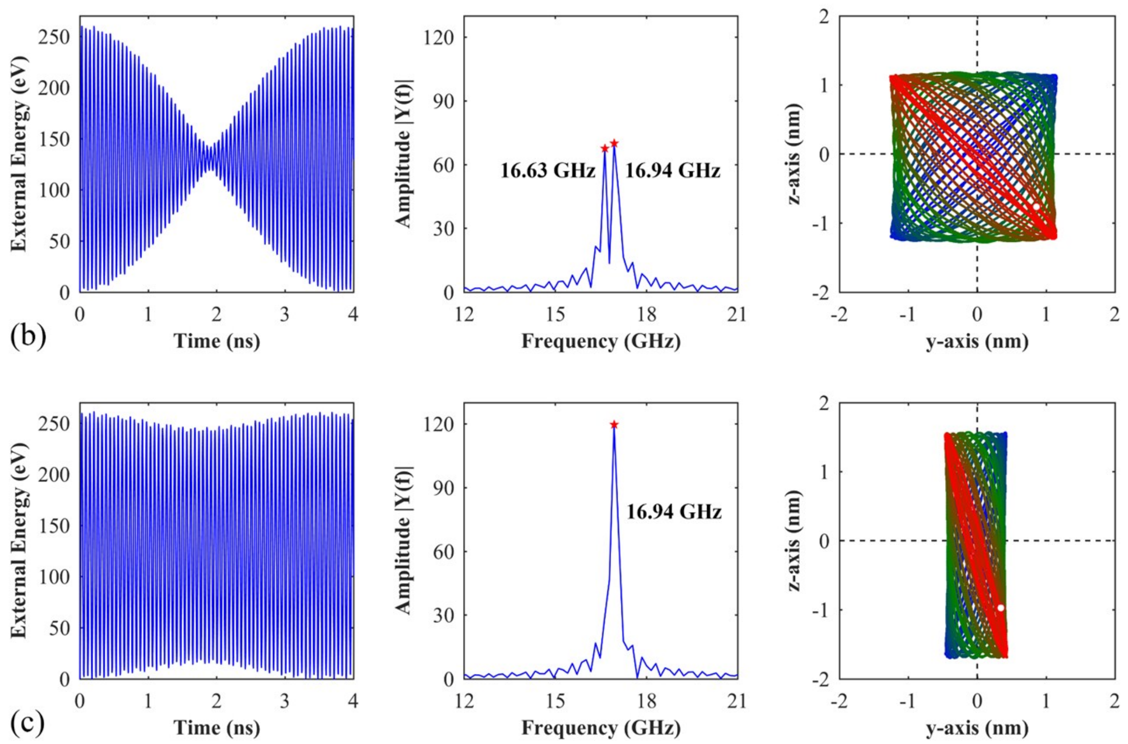


Figure S6. Vibrational behaviors of <110> orientated Si NW. The time history of the external energy (left panel), the corresponding frequency spectrum obtained from FFT analysis (middle panel), and the trajectory of the center of mass (right panel) for the NW under the excitation with an angle of: (a) 15°, (b) 45°, and (c) 75° with its orthogonal $[\bar{1}10]$ direction.

S6. Vibrational behaviors of cantilevered <110> Si NWs

As expected, the cantilevered <110> Si NW exhibit a dual mode vibration due to its directional dependent shear modulus. The two first-order natural frequency can be clearly distinguished from the frequency spectrum (**Figure S7**a), corresponding to the two-dimensional movement of the center of mass (**Figure S7**b).

Figure S7c and 7d shows the trajectory of the center of mass for the <110> Si NW under the excitation along its orthogonal directions, from which, the NW shows one single mode vibration. Figure S7e and 7f compares the corresponding time history of the kinetic energy during vibration. Assuming the quality factor Q is a constant during vibration, its value can be estimated based on $KE_n = KE_0(1-2\pi/Q)^n$, where KE_0 and KE_n are the initial maximum kinetic energy and the maximum kinetic energy after n vibration cycles. According the simulation results, a high Q around 3×10^8 and 6×10^8 are estimated for the vibration along the two orthogonal directions (i.e., $[\bar{1}10]$ and $[100]$), respectively.

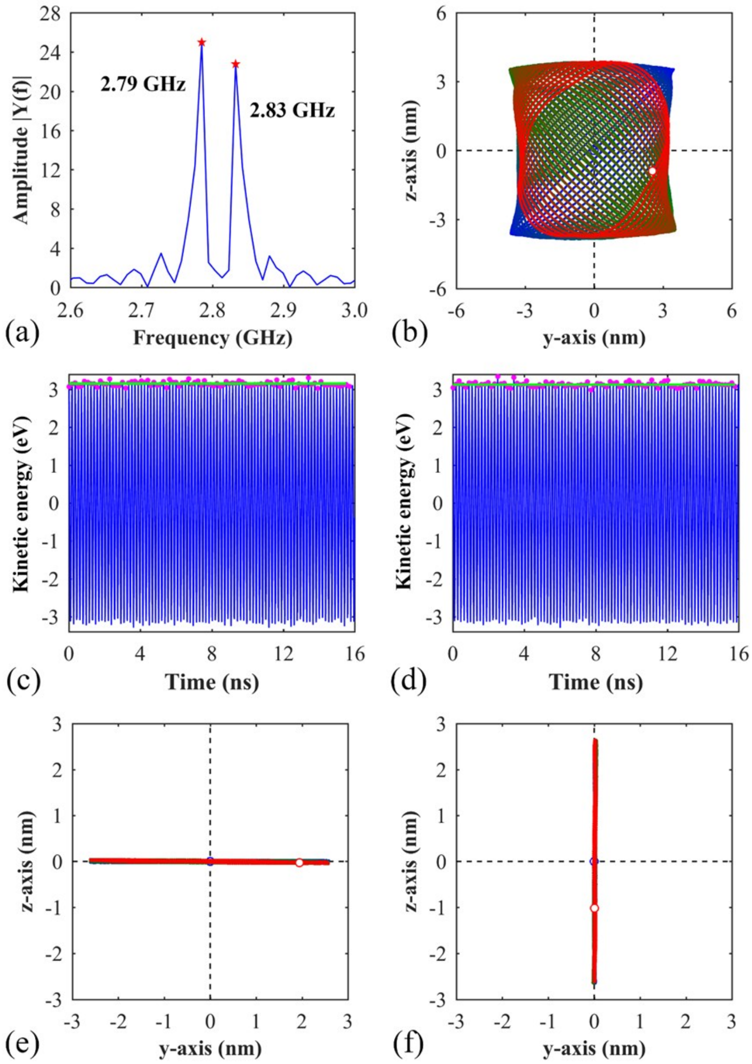


Figure S7. Vibrational behaviors of cantilevered <110> Si NW. (a) the frequency spectrum obtained from FFT analysis based on the time history of the displacement in Figure 8, and (b) the trajectory of the center of mass for the NW under the excitation with an angle of 45° with its orthogonal $[\bar{1}10]$ direction. The trajectory of the center of mass for the NW under the excitation along the two orthogonal directions: (c) $[\bar{1}10]$; and (d) $[100]$, and the corresponding time history of the displacement for the NW with the excitation along: (e) $[\bar{1}10]$; and (f) $[100]$. The NW here is actuated by an excitation in the form of $v(x) = 2a\cos^2(\pi(x-2L)/4L)$, mimicking a bent cantilever profile. Here, a equals to 0.5 Å. The green lines represent the fitting curve for the calculation of the quality factor, and the soild markers highlighted all peak values of the kinetic energy in each vibratin cycle.