Supporting Information for

Structural and electronic properties of $NaTaO_3$ cubic nanowires

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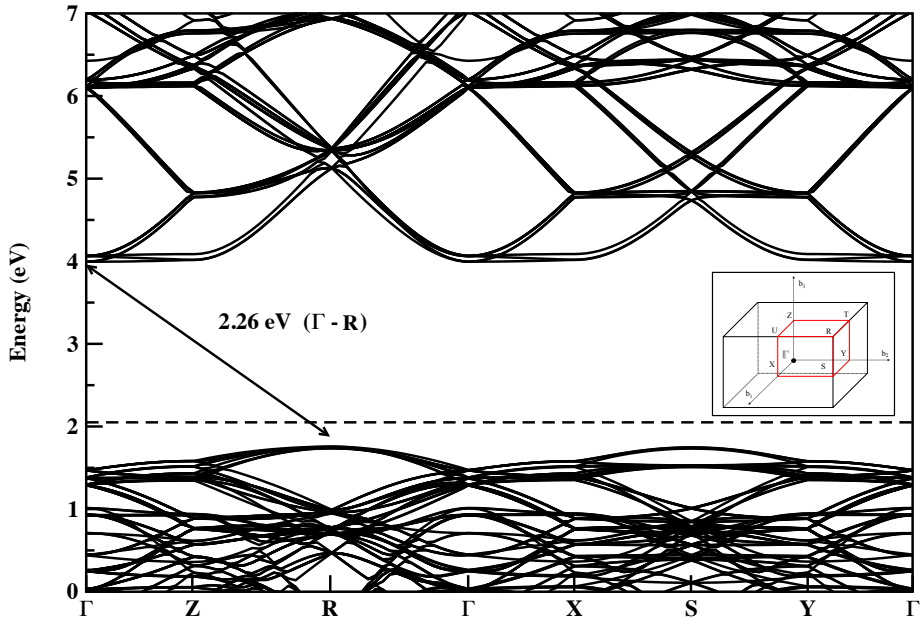

Figure 1S. $NaTaO_3$ cubic bulk band structure obtained through GGA (PBE) first-principles DFT calculations. The Fermi level (E_F) is represented by the black dashed line at 2.05 eV. The indirect band gap value of 2.26 eV in the Γ-R direction is indicated by the black arrow. We highlight the cubic first Brillouin zone in the inset in order to elucidate the R-Z folding which explains the energetic *memory* of the wires with respect to their growth direction.

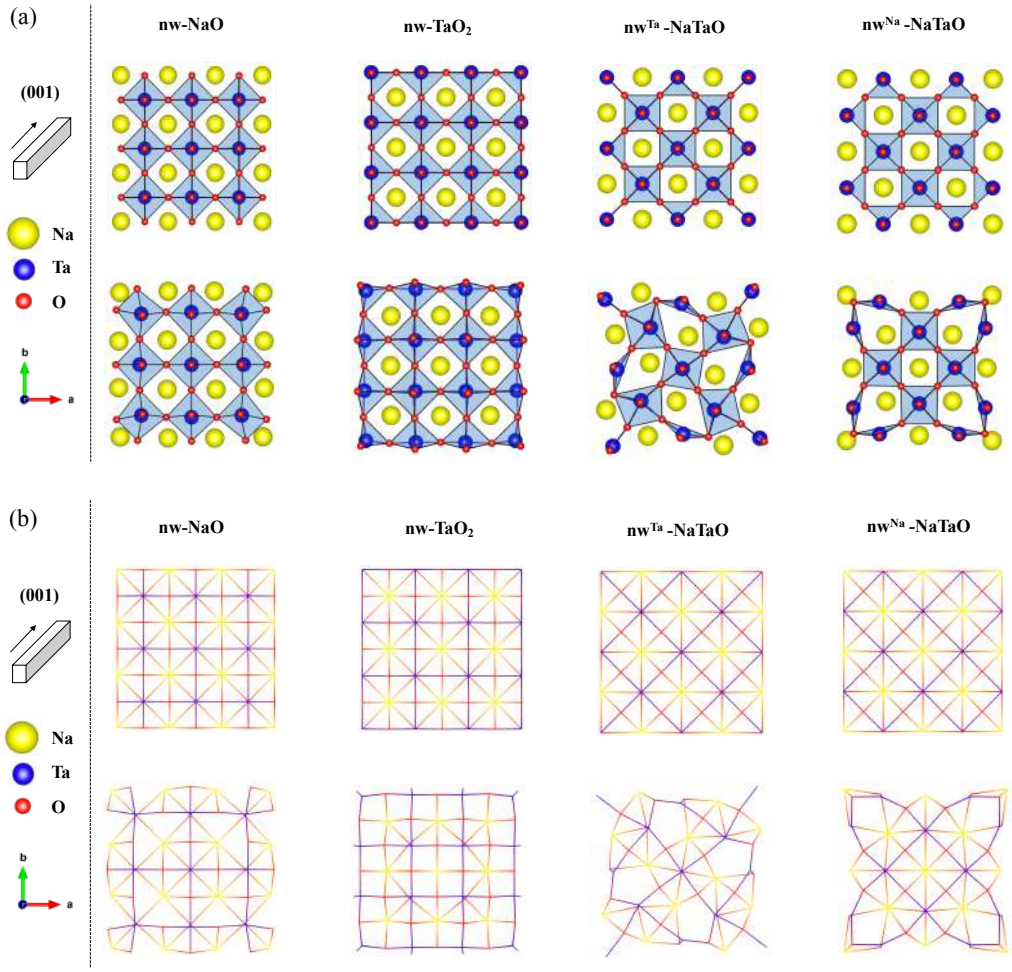

Figure 2S. Polyhedral (a) and wireframe (b) representations of initial (top) and relaxed (bottom) of all proposed $NaTaO_3$ nanowires. Polyhedral representations may better elucidate both the relaxation which takes place for nw-NaO and nw-TaO_2, as well as the reconstruction that modify $nw^{Ta,Na}$-NaTaO surface facets stoichiometry. In (b), Ta-O-Ta bond angle changes can be seen more explicitly, whereas surface TaO_4 rotation and O displacements are clearer in (a). Wireframe images reveal changes in the wires' symmetry after the equilibrium has been reached, which qualitatively pictures their resulting crystallinity.

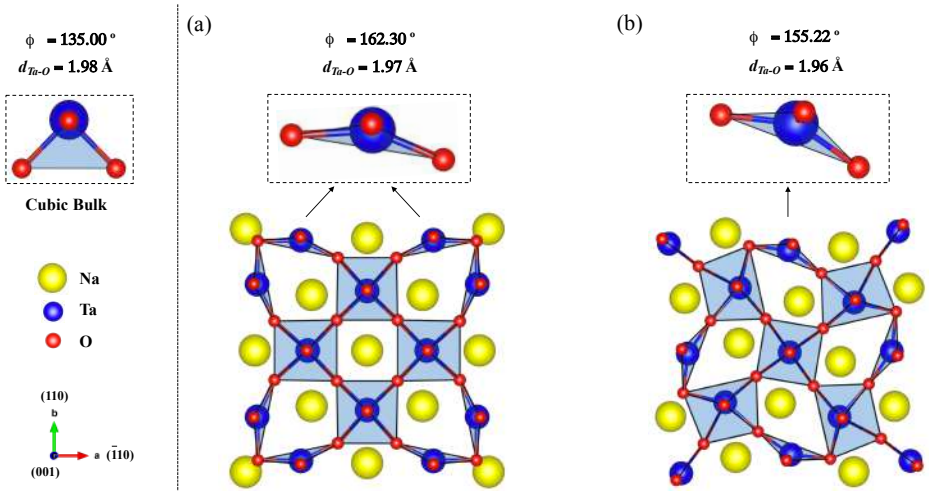

Figure 3S. Polyhedral representation of relaxed nw^{Na}-NaTaO (a) and nw^{Ta}-NaTaO (b). Surface TaO_4 units were highlighted to evidence their difference. The eight tetrahedra in nw^{Na}-NaTaO surface are more flexible than the four found in nw^{Ta}-NaTaO since they show a wider variation of O-Ta-O bond angles (ϕ) compared to the bulk. Besides that, they are also more planar, showing ϕ values closer to 180º.

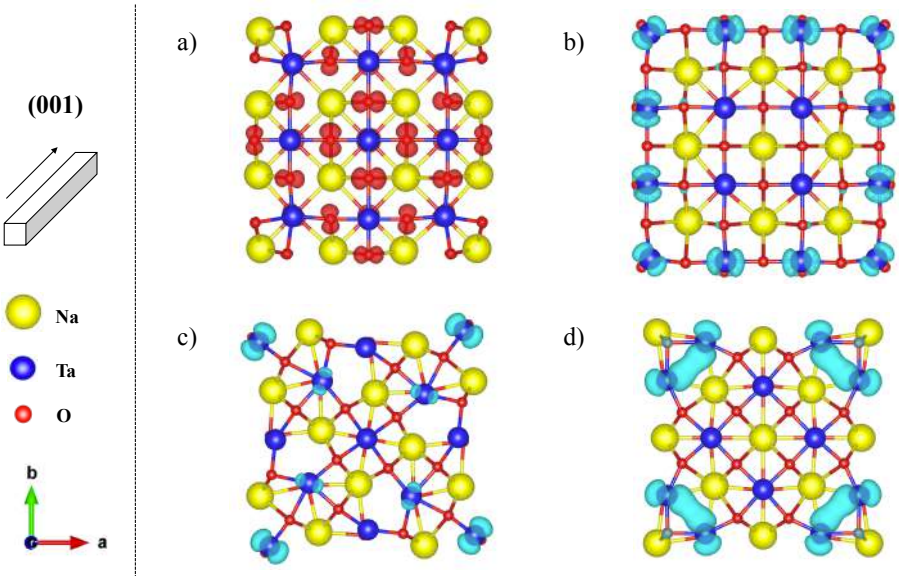

Figure 4S. Partial charge density around the Fermi level for all calculated nanowires. For nw-NaO (a), the charge density is delocalized all over its oxygen atoms except those from the edge whose contributions are mainly associated with localized states above the wire VB. The Fermi level vicinity of nw-TaO_2 (b) is delocalized all over its surface Ta *d* orbitals while for nw^{Ta}-NaTaO (c) and nw^{Na}-NaTaO (d) it is more localized on edge atoms. Interesting is the facet that a *d-d* overlap occurs again for nw^{Na}-NaTaO, which may be the reason why such E_F is the smallest in energy. An isosurface value of 0.005 e/$Borh^{-3}$ was used for all four plots. The Fermi level vicinity was defined as 0.01 eV above and below it. The results are consistent with the pDOS plot.

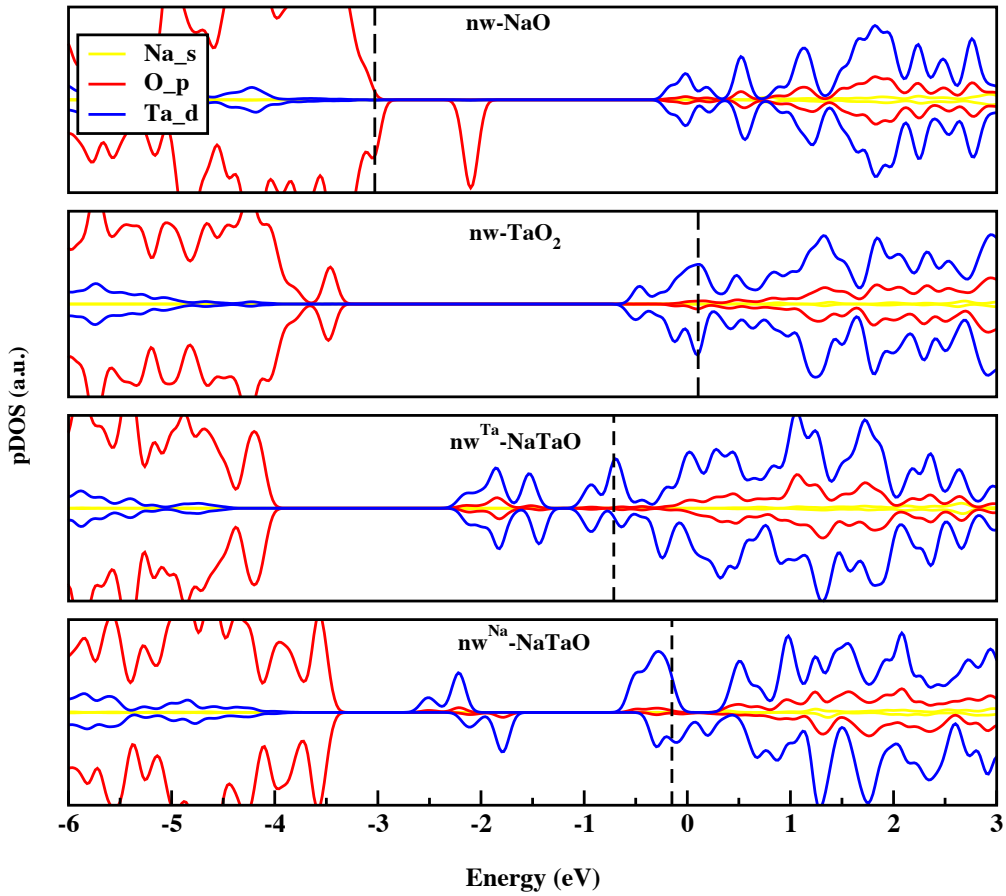

Figure 5S. Projected density of states for all the proposed nanowires with spin-orbit interaction calculations (SOC). As tantalum is a transition metal with completely filled 4*d* and 4*f* layers as well as partly filled 5*d* orbitals, SOC may well alter the electronic structure of the wires and cause the splitting of spin up and down states. However, we see that it was not the case for the proposed wires since only slight changes occurred mainly for the ones exposing Ta on their surface, as expected. Localized levels within the gap for nw-NaO and $nw^{Ta,Na}$-NaTaO kept their character with no significant changes.