Support Information

Stability of NNO and NPO Nanotube Crystals

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Figure S1

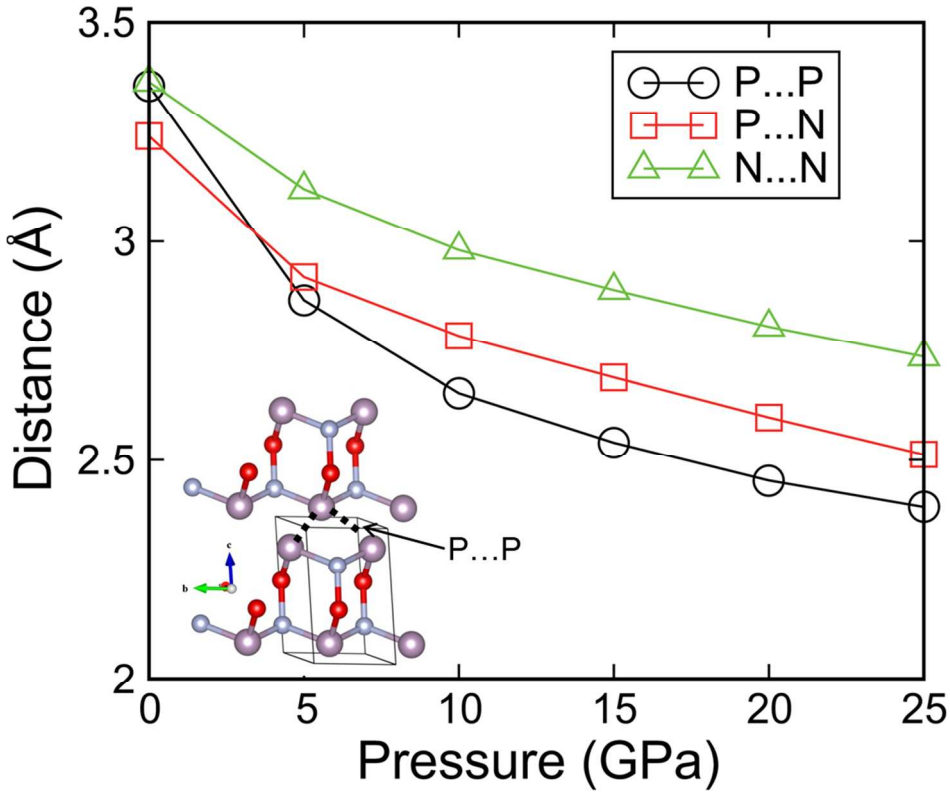

Figure S1. Non-bond distances P…P, P…N and N…N in NPO nanotube crystal as a function of pressures. Each P forms two P…P of equal distance with two P in the nearby nanotube. The six member ring of the tube is not parallel to the xz plane (tube axis is y direction). Actually they have one NOP parallel to xz plane in one side, then another NOP are also parallel to xz plane but shift ~0.8 A of the y direction in the other side. Then these two NOP molecules are connected by two NP bonds to form the six member ring. Thus one NOP is in the middle (y direction) of two NOP of the nearby tube when two nanotubes are getting close. The insert shows the configurations with nearby nanotube at 25 GPa.

Figure S2

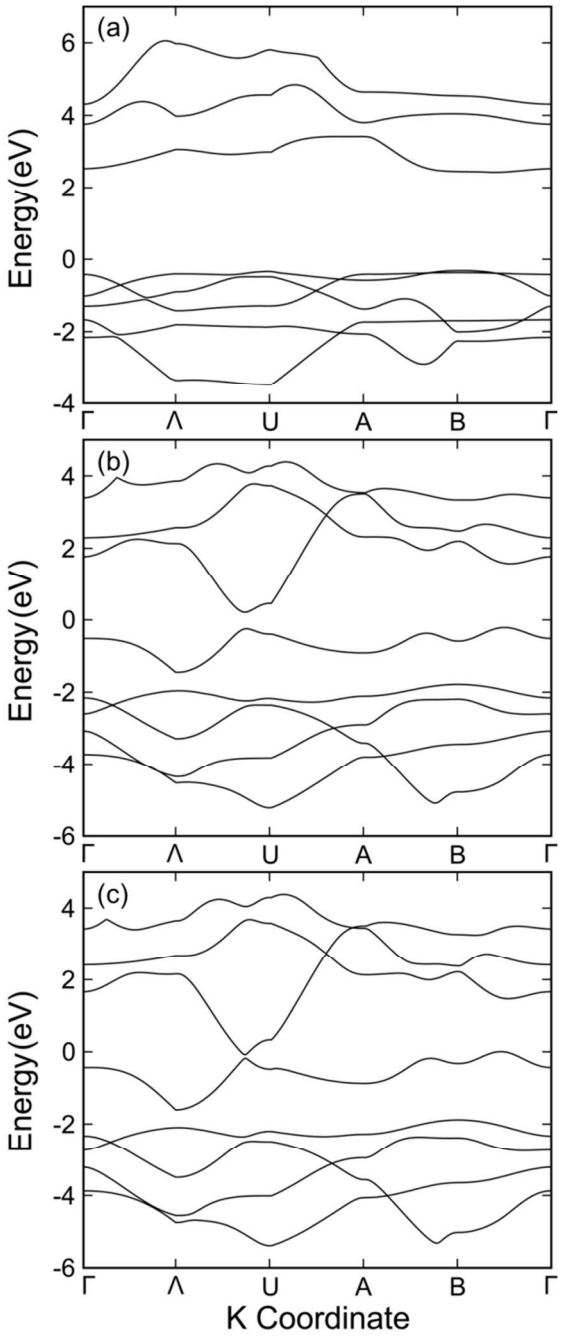

Figure S2. The band structures of NPO tube at various pressures along Γ(0,0,0)→Λ(0,1/4,0)→U(1/2,1/4,1/2)→A(1/2,0,1/2)→B(1/2,0,0)→Γ(0,0,0) in reciprocal space: (a) P = 0 GPa, (b) P = 20 GPa, and (c) P = 25 GPa. The pressure stabilizes the LUMO near the U point as pressure increase because of the P lone pair overlaps between two nearby nanotubes.

Figure S3

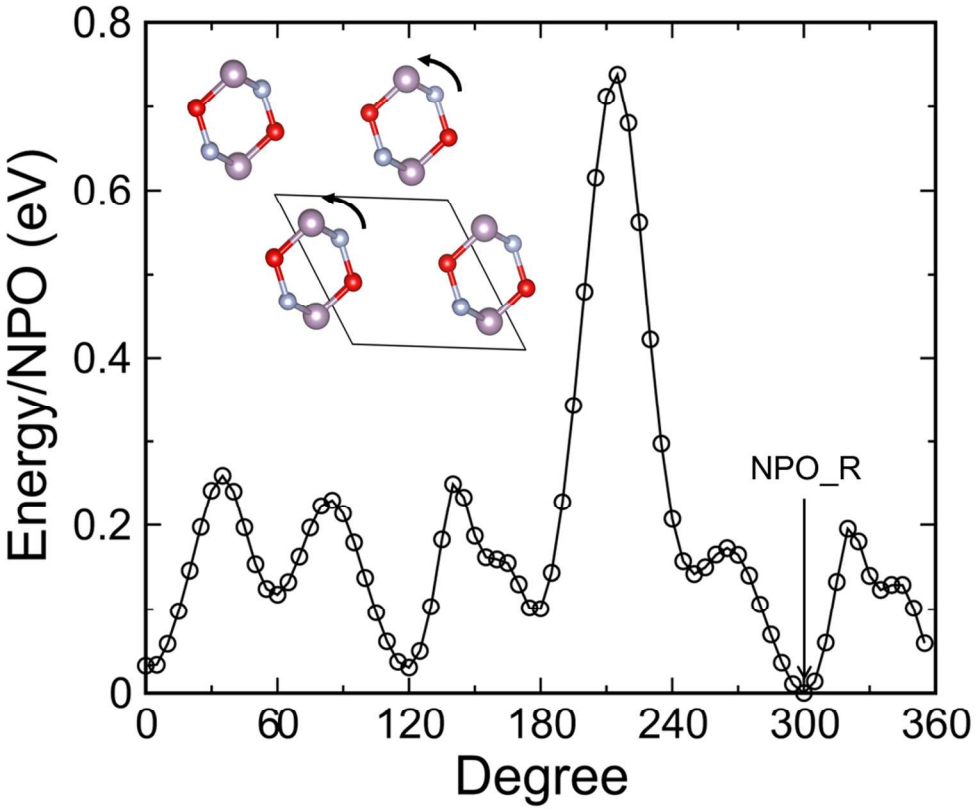

Figure S3. Potential energy curve of rotating the nearby nanotube under counterclockwise direction. Several local minimum appears. The global minimum structure is rotate 60 degree clockwise (NPO_R). The same orientation tube is the second lowest energy.

Figure S4.

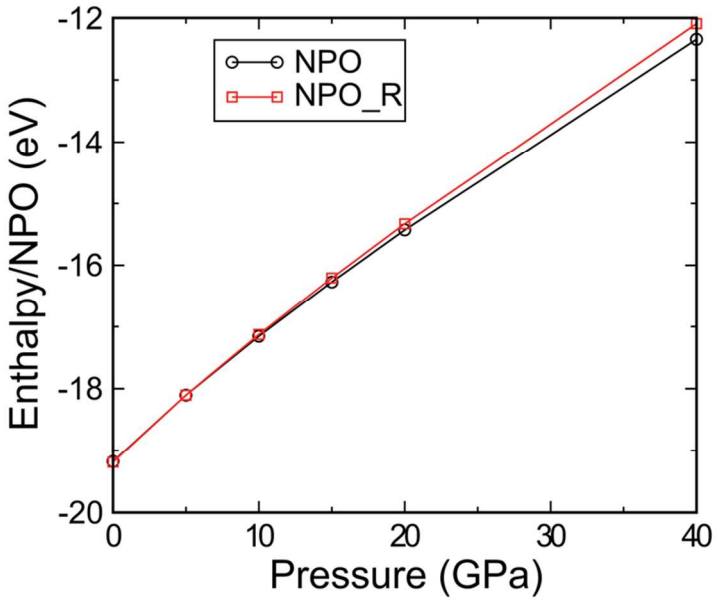

Figure S4. The enthalpy of NPO and NPO_R structures as a function of pressure. The NPO structure with the same tube orientation is more favorite above 10 GPa.

Figure S5.

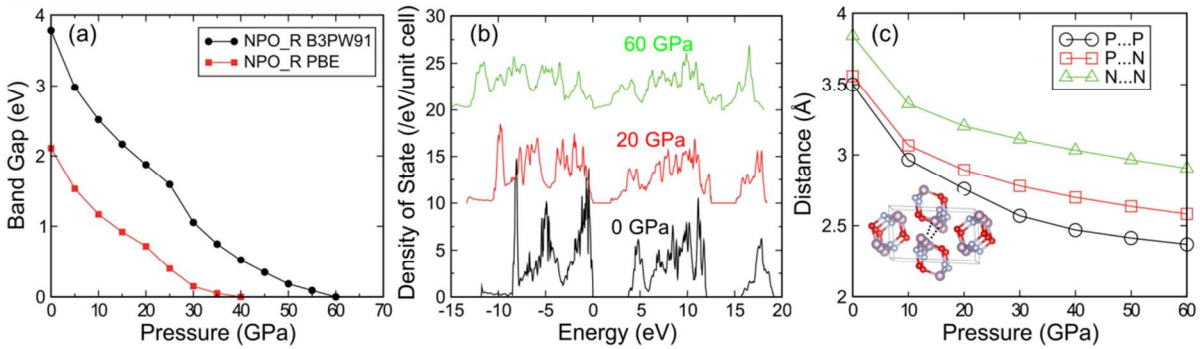

Figure S5. Electronic properties of NPO_R tube structure as a function of pressure. (a) The band gap decreases as pressure increases, the metallic phase transition happened at 40 GPa for PBE and 60 GPa for B3PW91. (b) The electronic density of states at various pressures for B3PW91. (c) The non-bond distance P…P, P…N and N…N. The P…P non bond distance decrease from 3.50 Å to 2.37 Å (7% longer than P-P single bond) as pressure increased to 60 GPa, leading to metallic phase transition.