Supporting Information

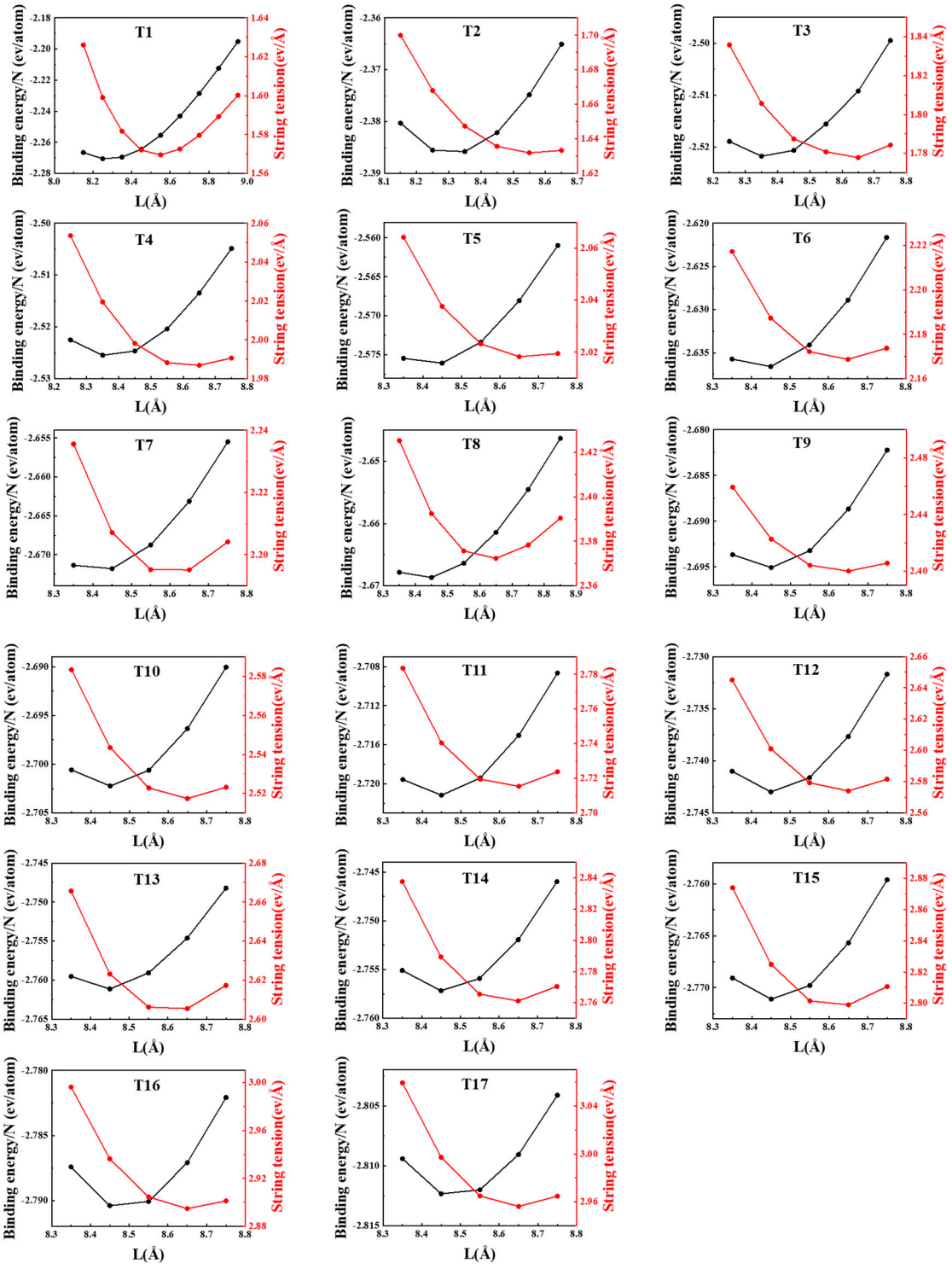
Ultra-thin gold nanowires

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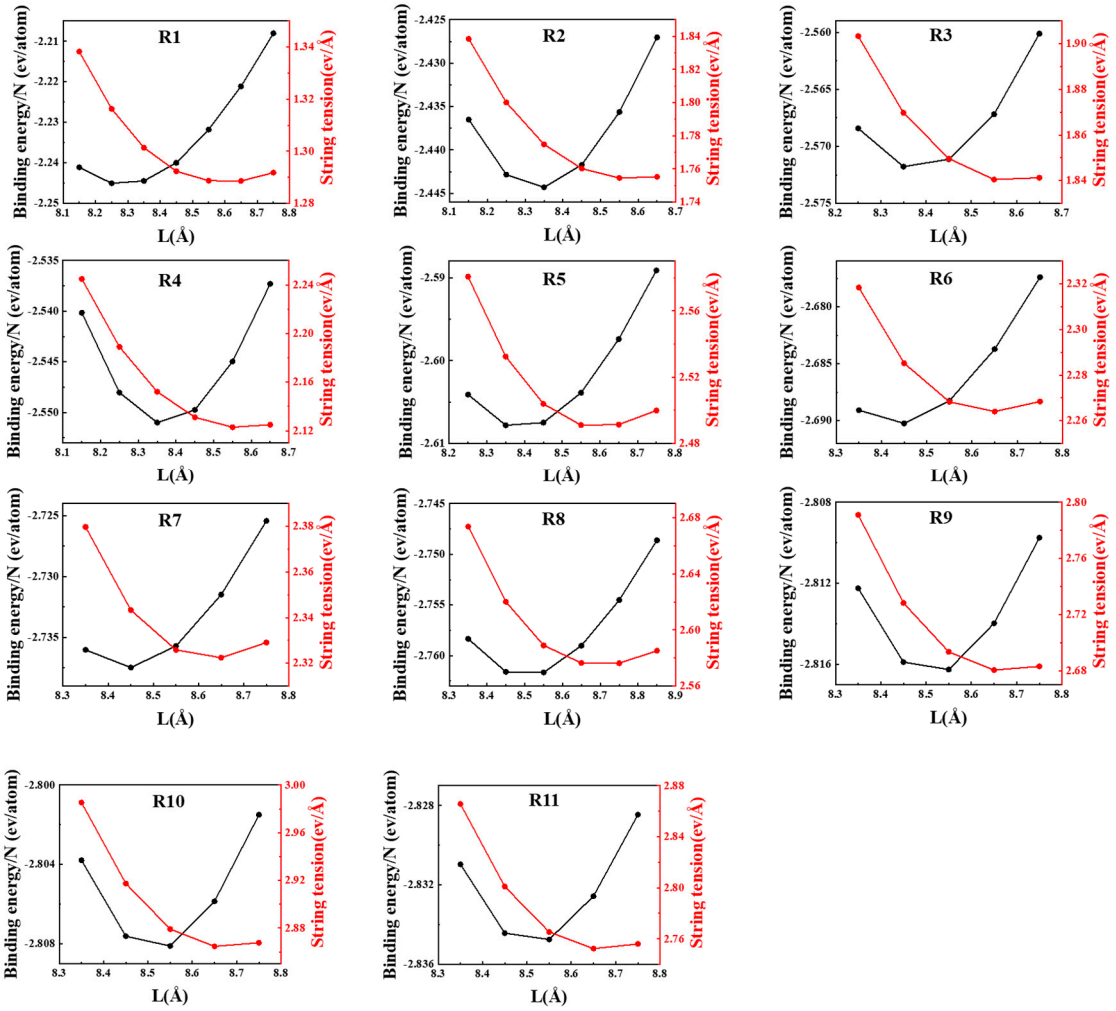
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Supporting Figures

(a)



(b)


R1
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R2
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R3
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R4
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R5
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R6
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R7
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R8
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R9
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R10
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)
R11
Binding energy/N (ev/atom)
String tension(ev/Å)
L(Å)

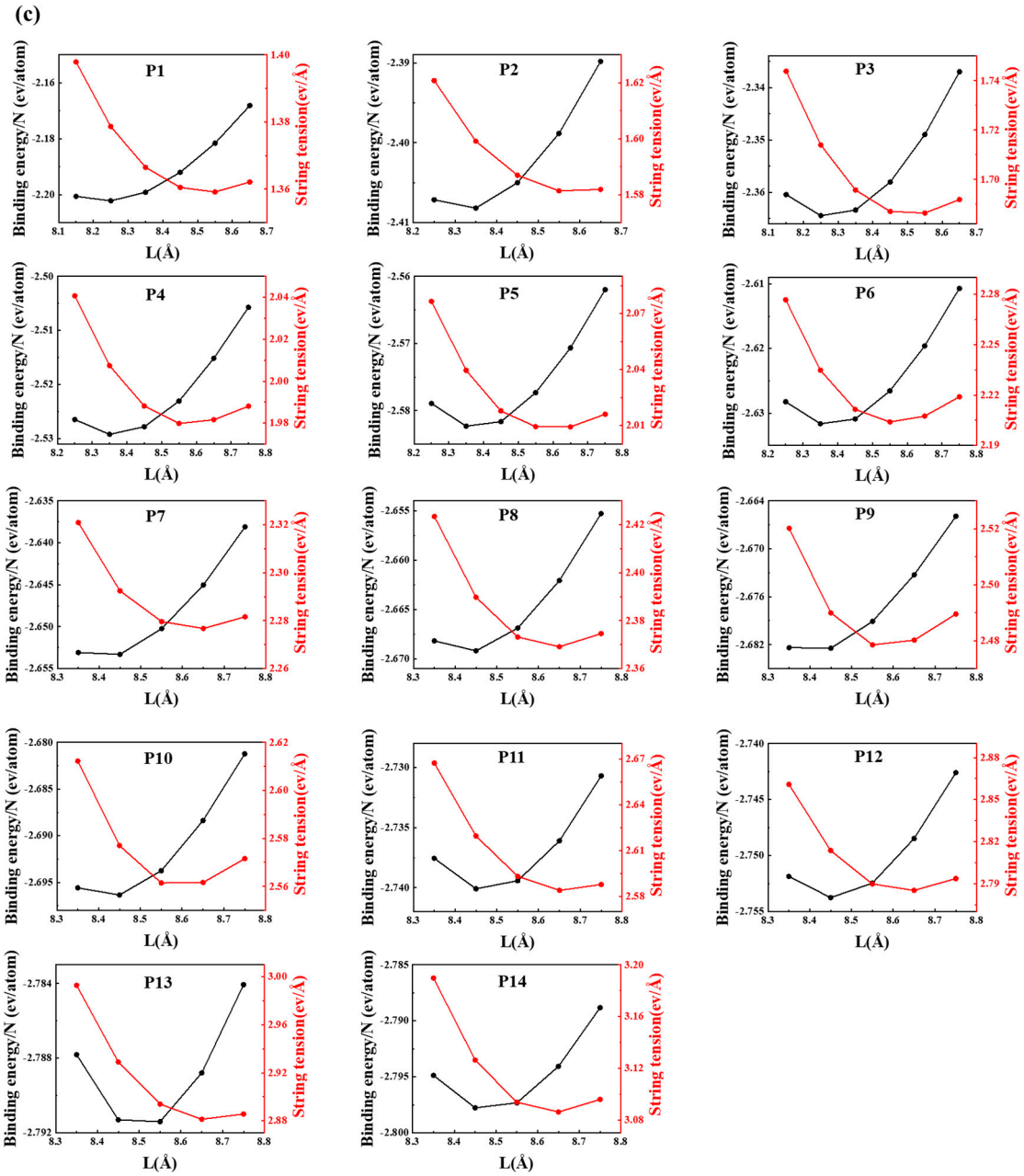


Figure S1. Calculated binding energy/N (left) and string tension/N (right) for Au NWs with different lengths (L) and cross-sectional structures: (a) T series, (b) R series, and (c) P series.

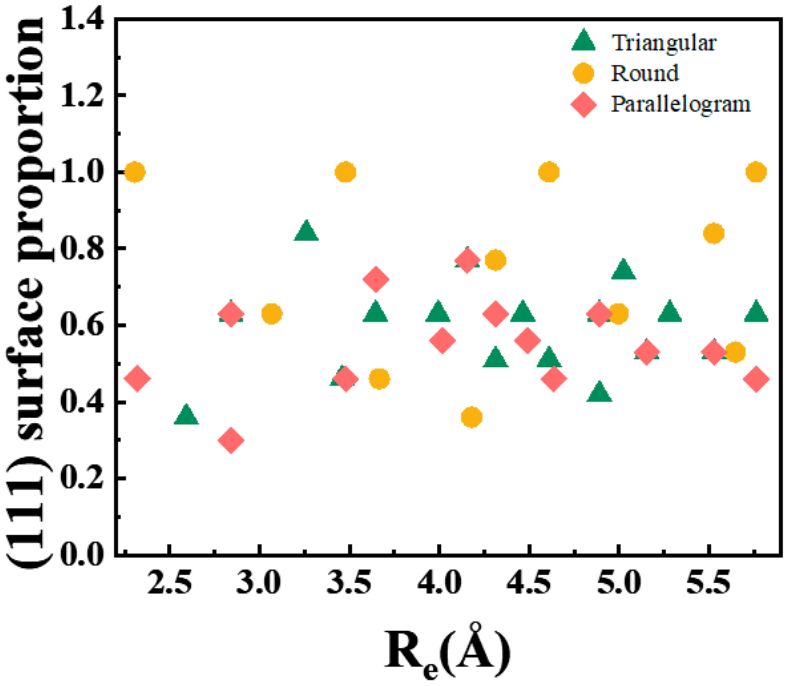
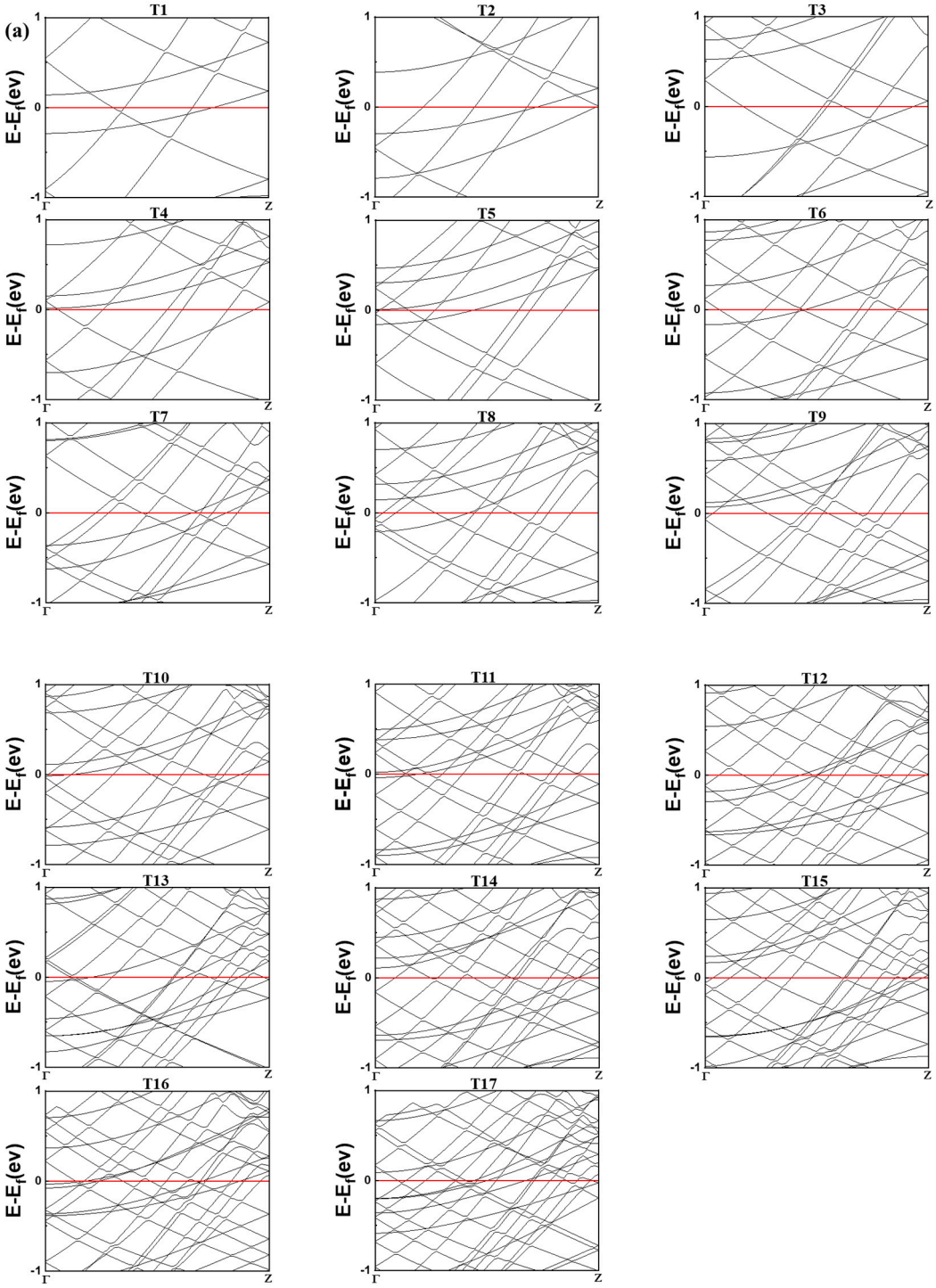
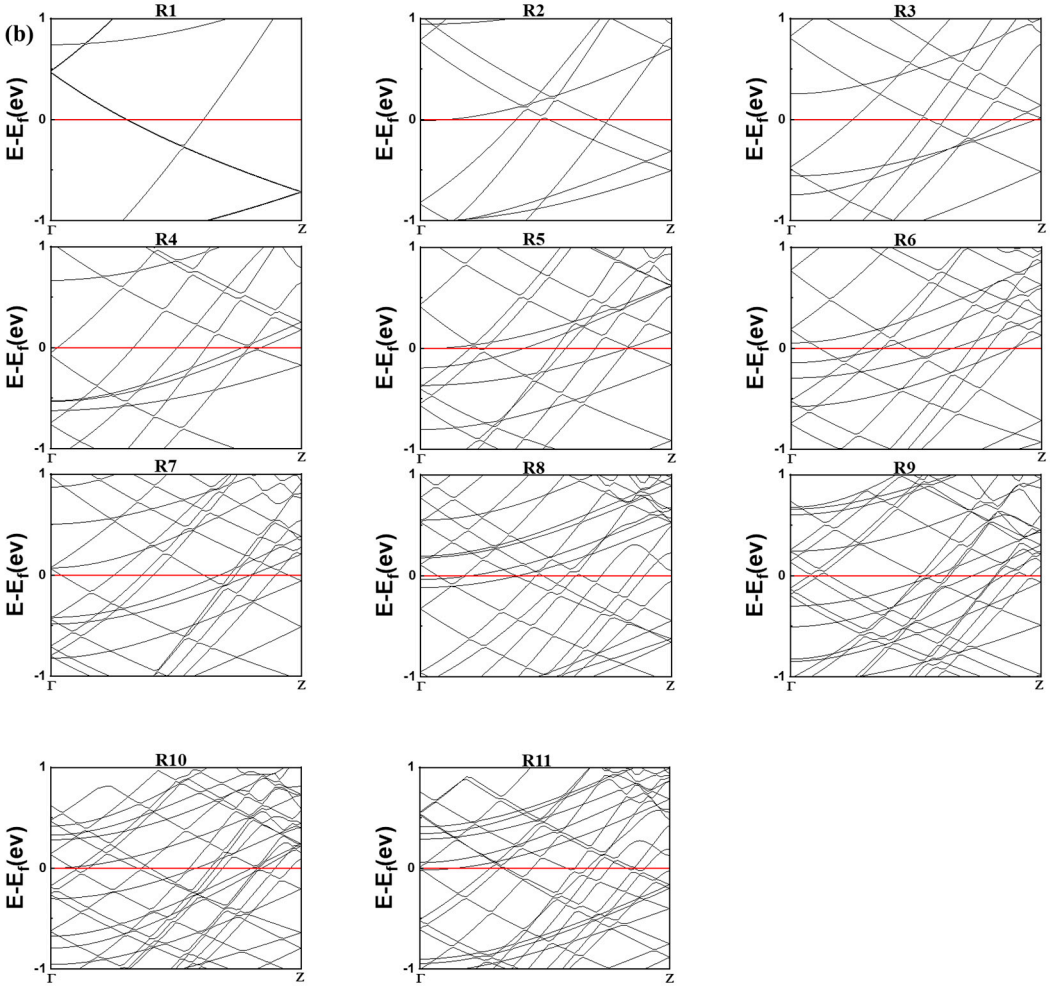


Figure S2. The proportion of (111) surface for the T, R, and P series.


(a)
T1
T2
T3
T4
T5
T6
T7
T8
T9
T10
T11
T12
T13
T14
T15
T16
T17
E-E$_f$(ev)
1
0
-1
Γ
Z


(b)
R1
R2
R3
R4
R5
R6
R7
R8
R9
R10
R11
E-E_f(ev)
1
0
-1
Γ
Z

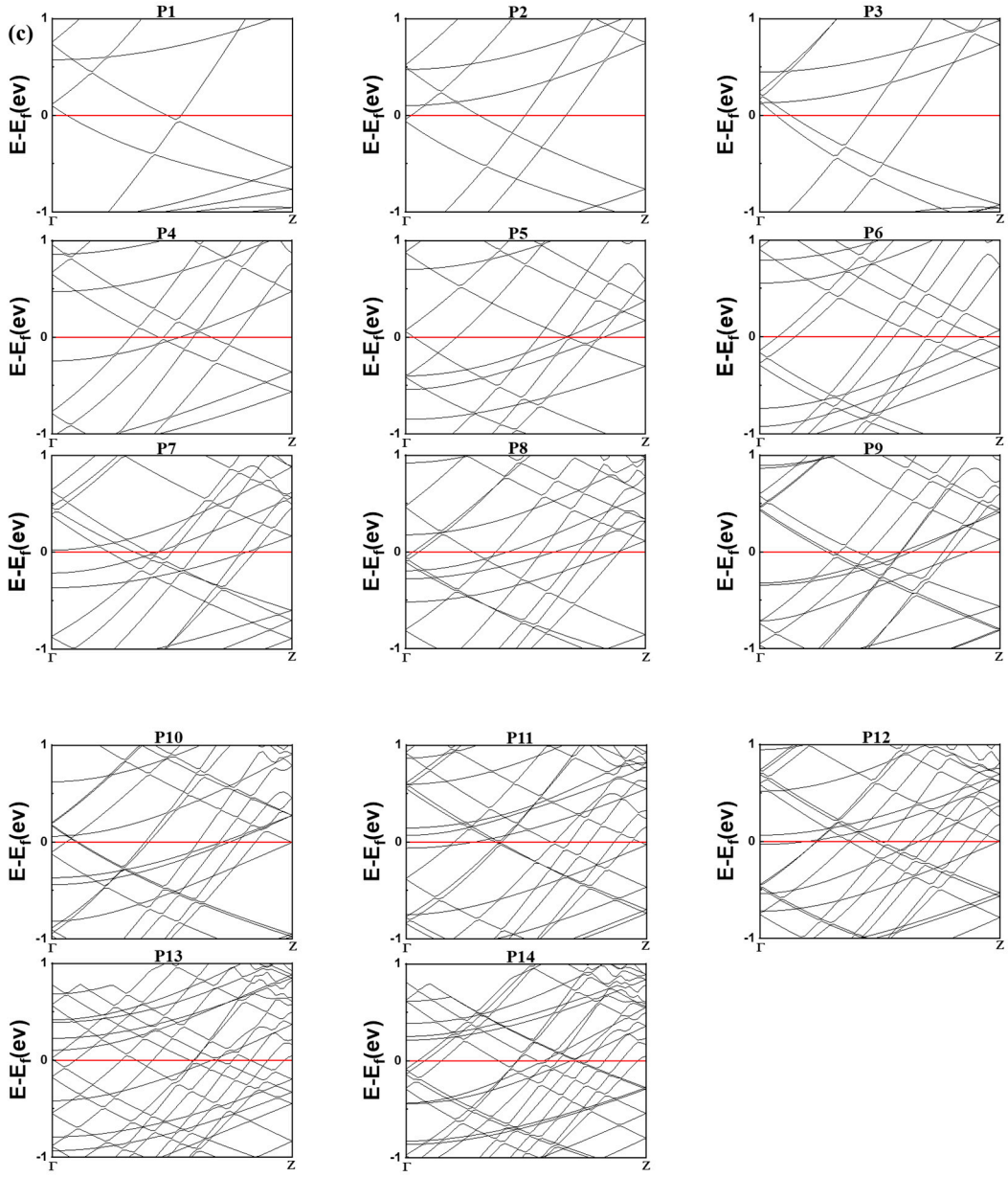


Figure S3. Calculated band structures of Au NWs cross-sections with different lengths (L) for the (a) T, (b) R, and (c) P series, respectively.