

## Supporting Information

### **Mechanically Controllable Conductance in Carbon Nanotube Based Nanowire**

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In our calculation, we have used different force criterion of 0.05 eV/Å and 0.02 eV/Å to optimized the structure of device with high pressure squashed CNT electrodes (molecular junction M5). Similar configurations are obtained. Furthermore, the transmission spectra of two structures are calculated. The results show that they are almost in the same profile (see the following Fig. S1). Therefore, 0.05 eV/Å is adopted as the force convergence criterion in our calculation to balance the accuracy and the calculation efficiency.

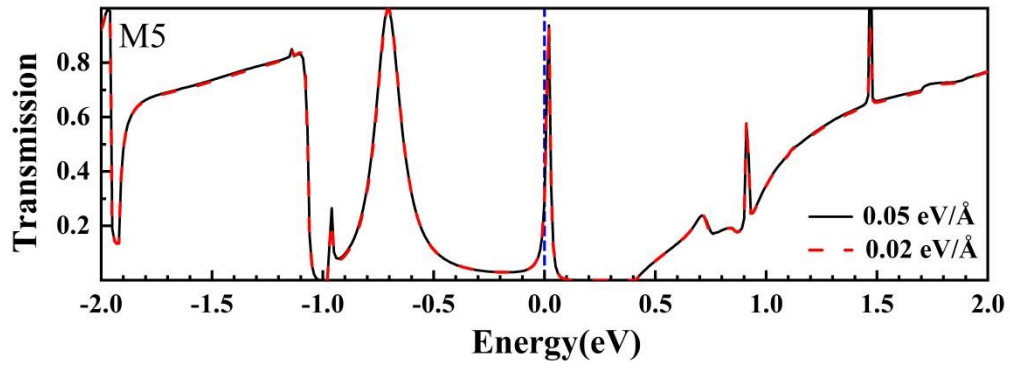


Fig. S1. Transmission spectra of molecular junction M5 under the force convergence criterion of 0.05 eV/Å and 0.02 eV/Å.

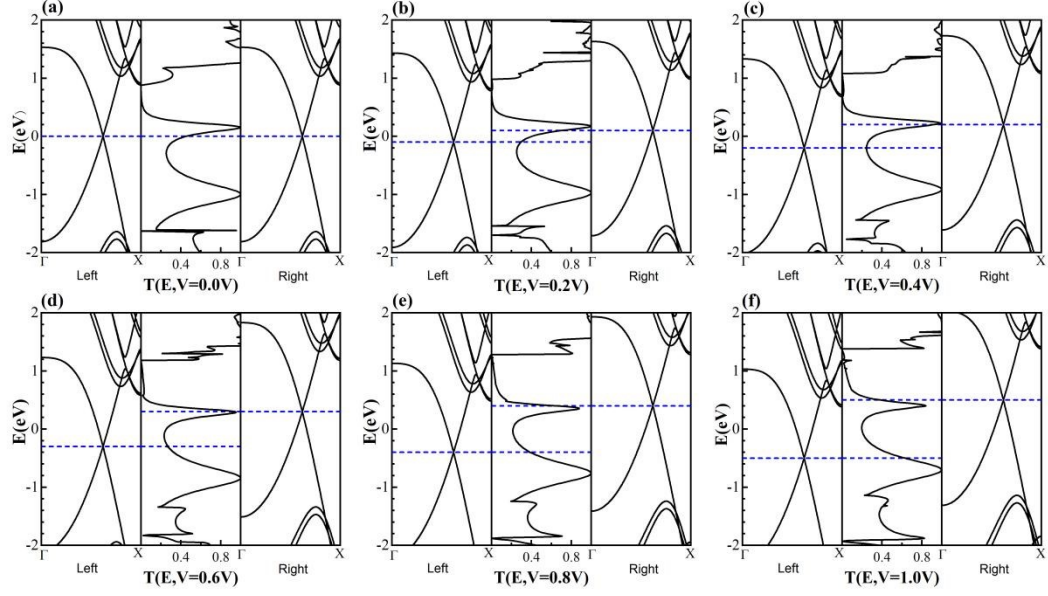


Fig. S2. Transmission spectra and band structures of both electrodes for M1 at (a) 0.0 V, (b) 0.2 V, (c) 0.4 V, (d) 0.6 V, (e) 0.8 V, and (f) 1.0 V.

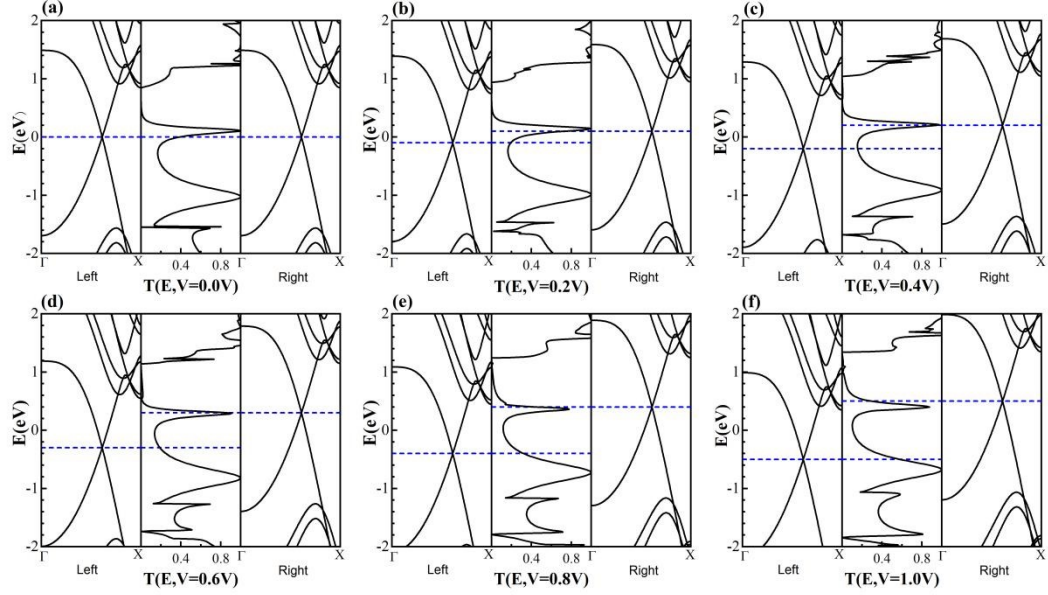


Fig. S3. Transmission spectra and band structures of both electrodes for M2 at (a) 0.0 V, (b) 0.2 V, (c) 0.4 V, (d) 0.6 V, (e) 0.8 V, and (f) 1.0 V.

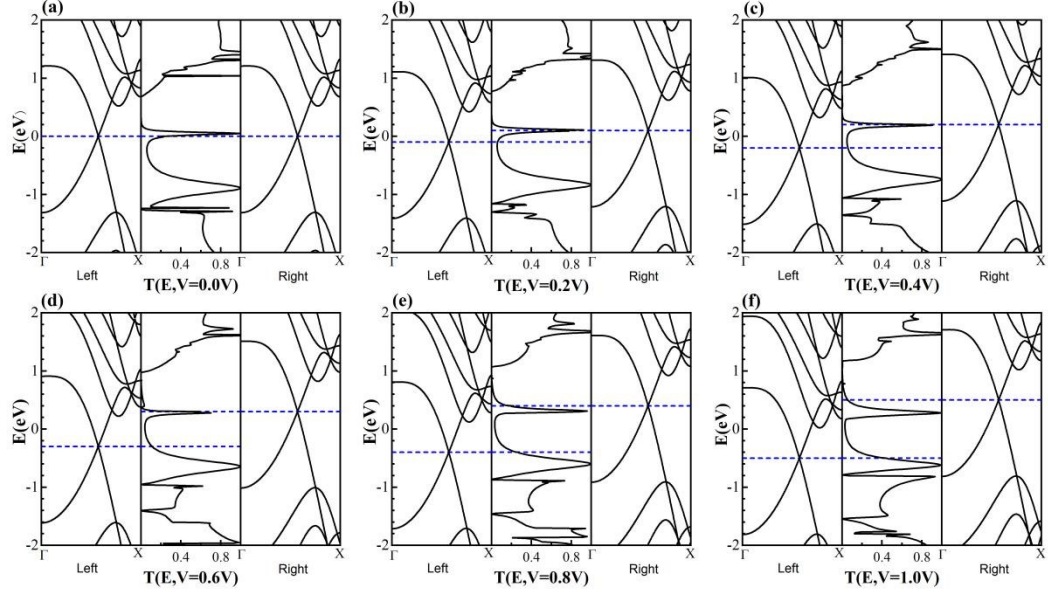


Fig. S4. Transmission spectra and band structures of both electrodes for M4 at (a) 0.0 V, (b) 0.2 V, (c) 0.4 V, (d) 0.6 V, (e) 0.8 V, and (f) 1.0 V.

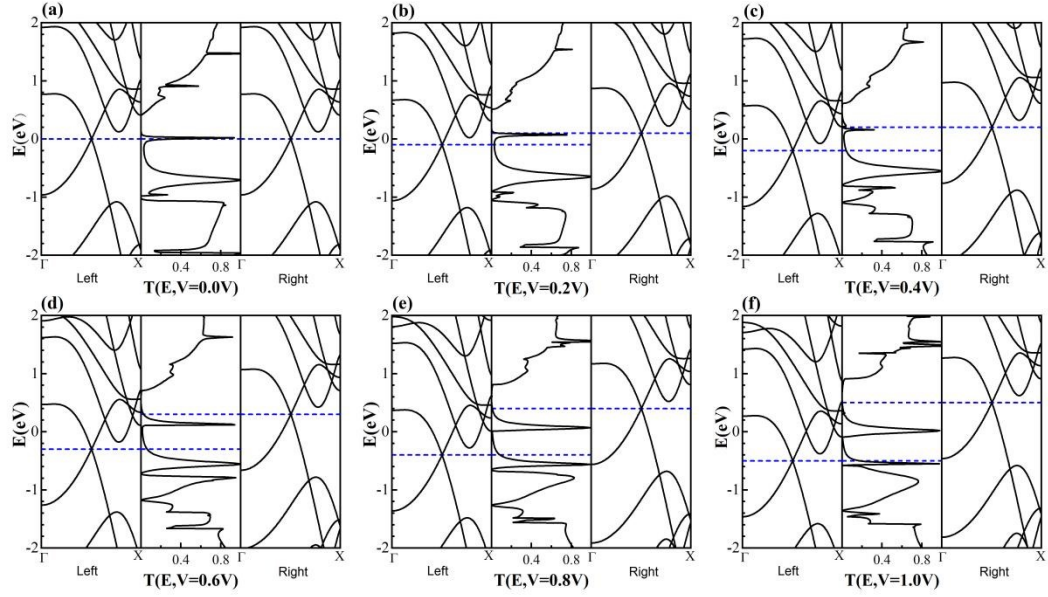


Fig. S5. Transmission spectra and band structures of both electrodes for M5 at (a) 0.0 V, (b) 0.2 V, (c) 0.4 V, (d) 0.6 V, (e) 0.8 V, and (f) 1.0 V.

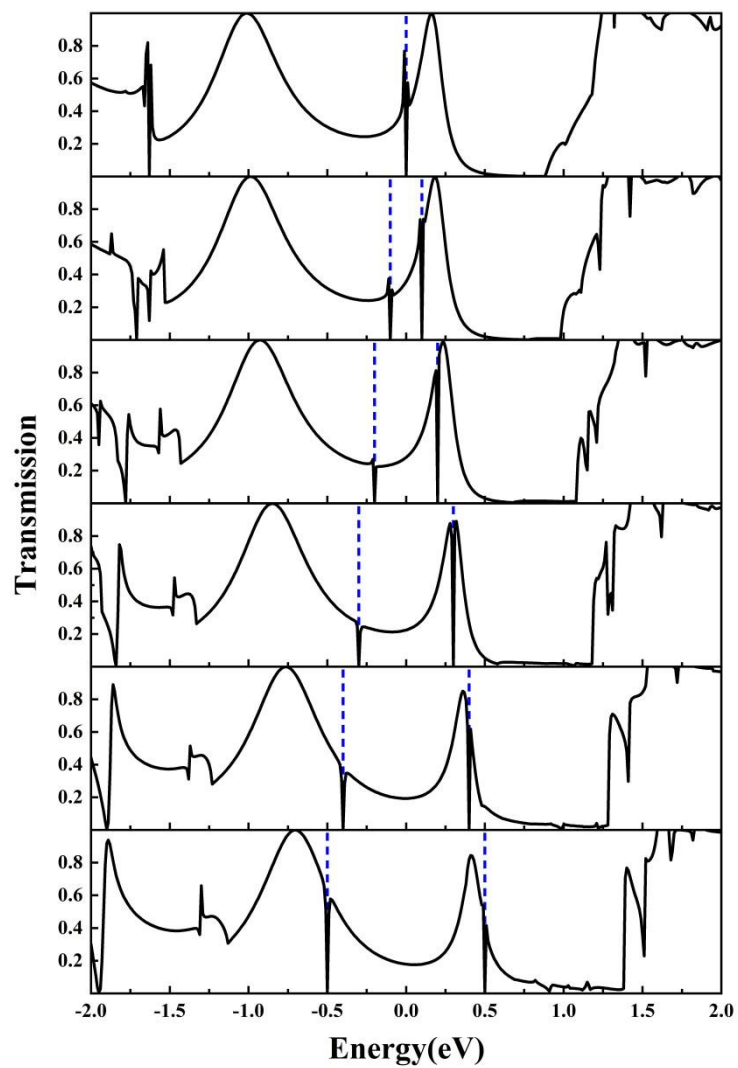


Fig. S6. Transmission spectra of molecular junctions for N1 at 0.0 V, 0.2 V, 0.4 V, 0.6 V, 0.8 V, and 1.0 V.

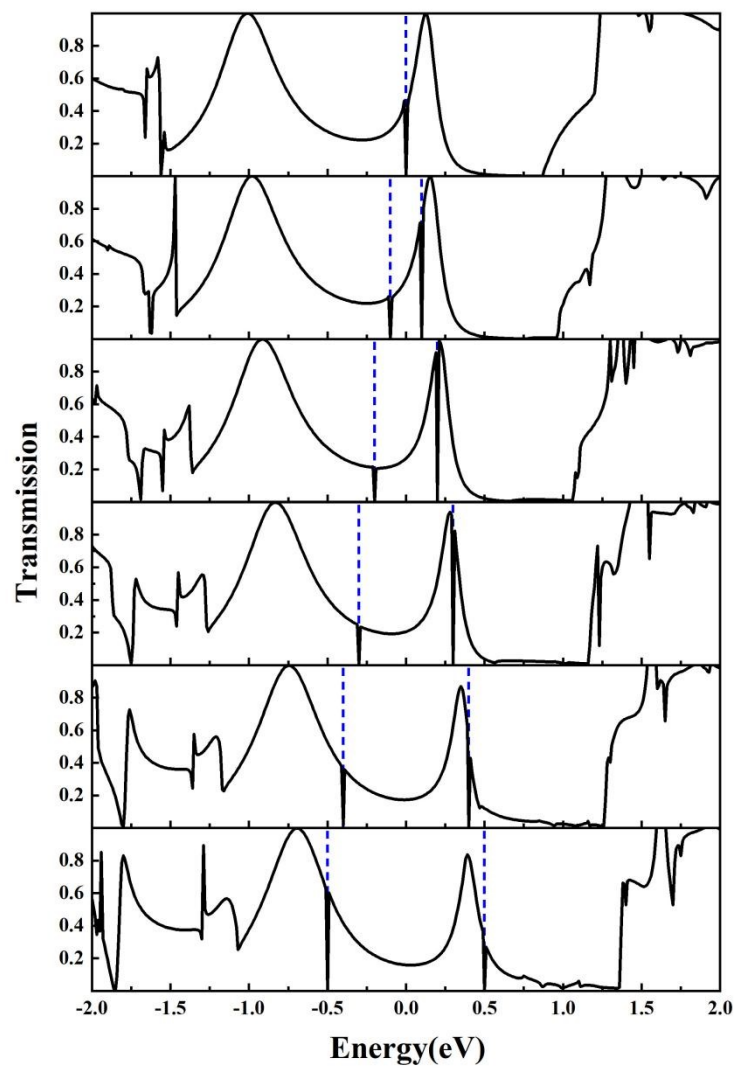


Fig. S7. Transmission spectra of molecular junctions for N2 at 0.0 V, 0.2 V, 0.4 V, 0.6 V, 0.8 V, and 1.0 V.

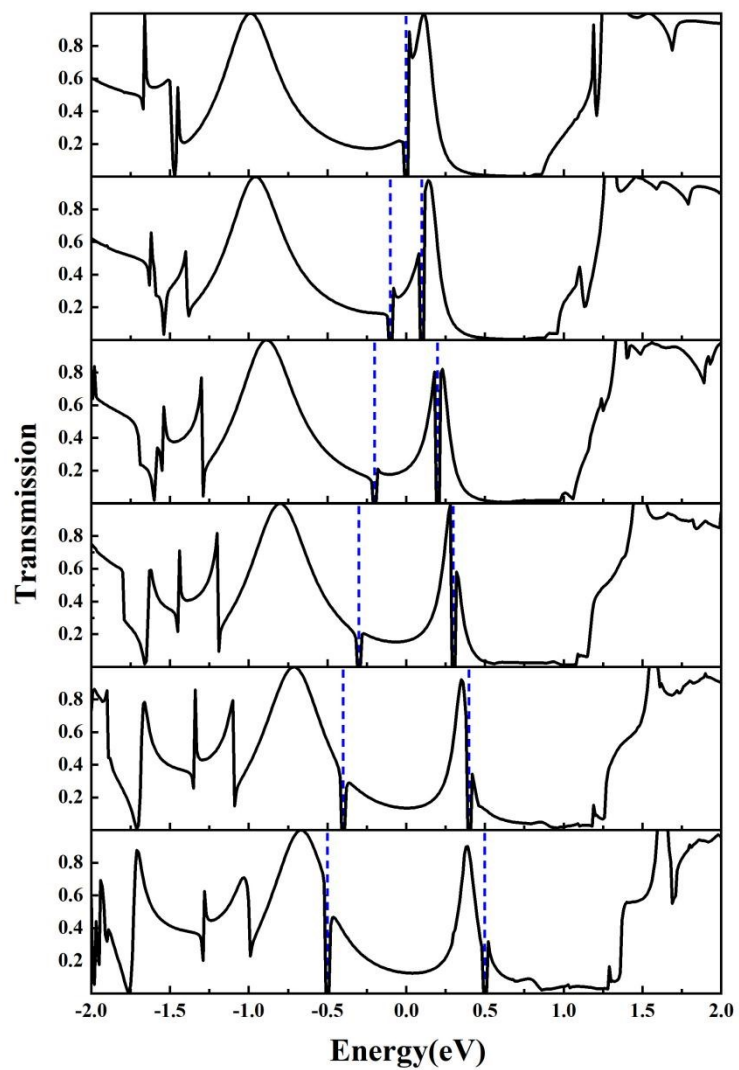


Fig. S8. Transmission spectra of molecular junctions for N3 at 0.0 V, 0.2 V, 0.4 V, 0.6 V, 0.8 V, and 1.0 V.

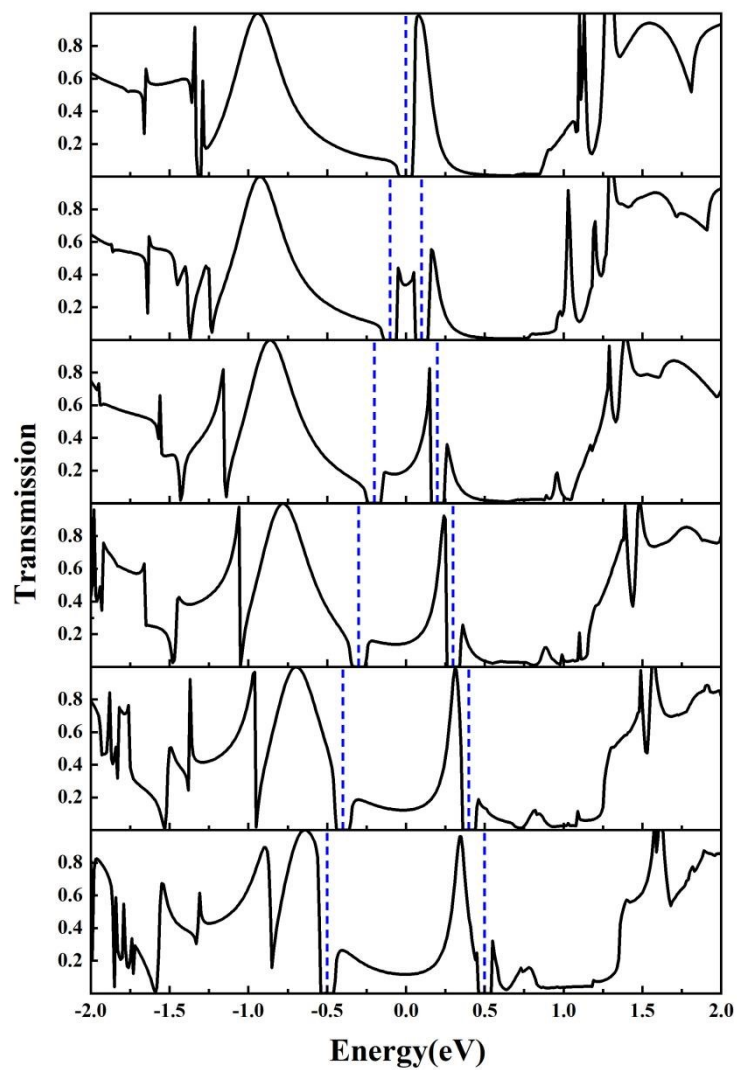


Fig. S9. Transmission spectra of molecular junctions for N4 at 0.0 V, 0.2 V, 0.4 V, 0.6 V, 0.8 V, and 1.0 V.

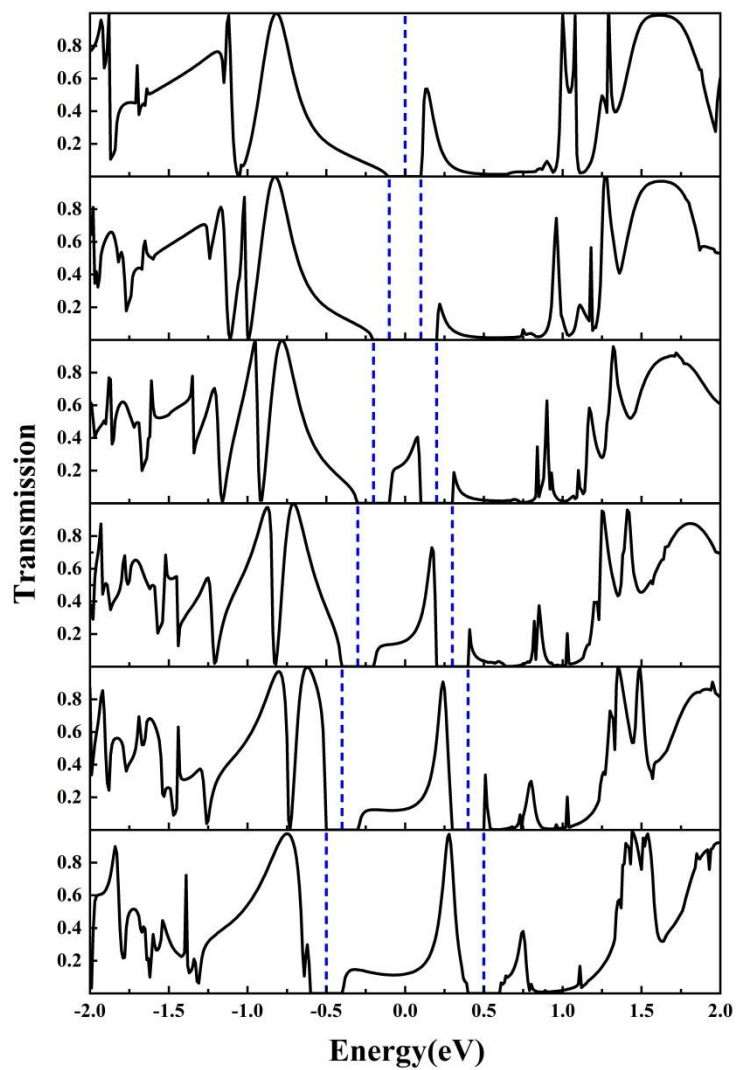


Fig. S10. Transmission spectra of molecular junctions for N5 at 0.0 V, 0.2 V, 0.4 V, 0.6 V, 0.8 V, and 1.0 V.

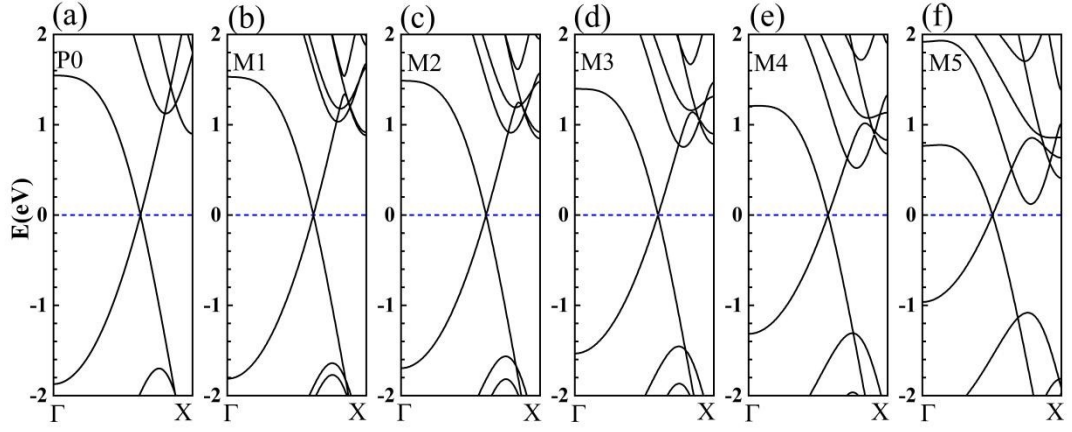


Fig. S11. Band structures of electrodes in (a) P0, (b) M1, (c) M2, (d) M3, (e) M4, and (f) M5 at zero bias. The blue dashed line indicates the Fermi level.

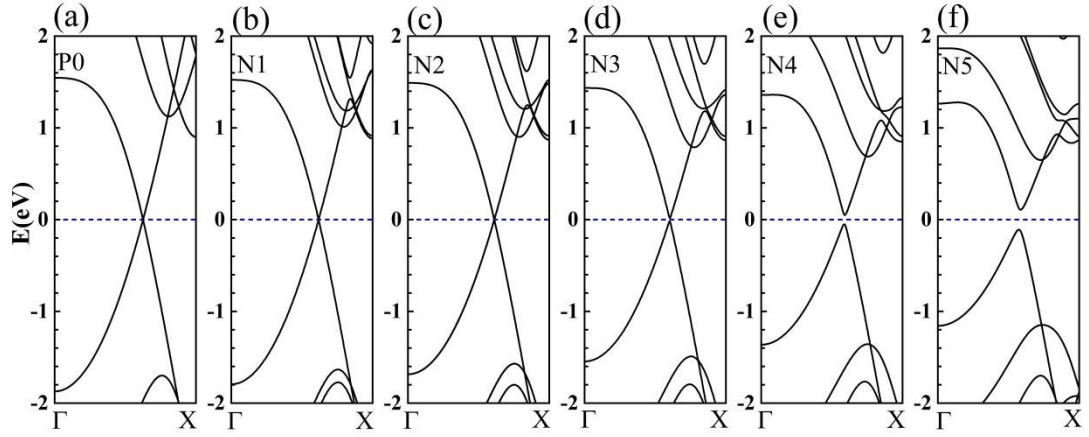


Fig. S12. Band structures of electrodes in (a) P0, (b) N1, (c) N2, (d) N3, (e) N4, and (f) N5 at zero bias. The blue dashed line indicates the Fermi level.