Electronic Supplementary Information for

Bias and molecular-length dependent odd-even effect of rectification in 4′-methyl-2,2′-bipyridyl-terminated *n*-alkanethiolate single-molecule diodes

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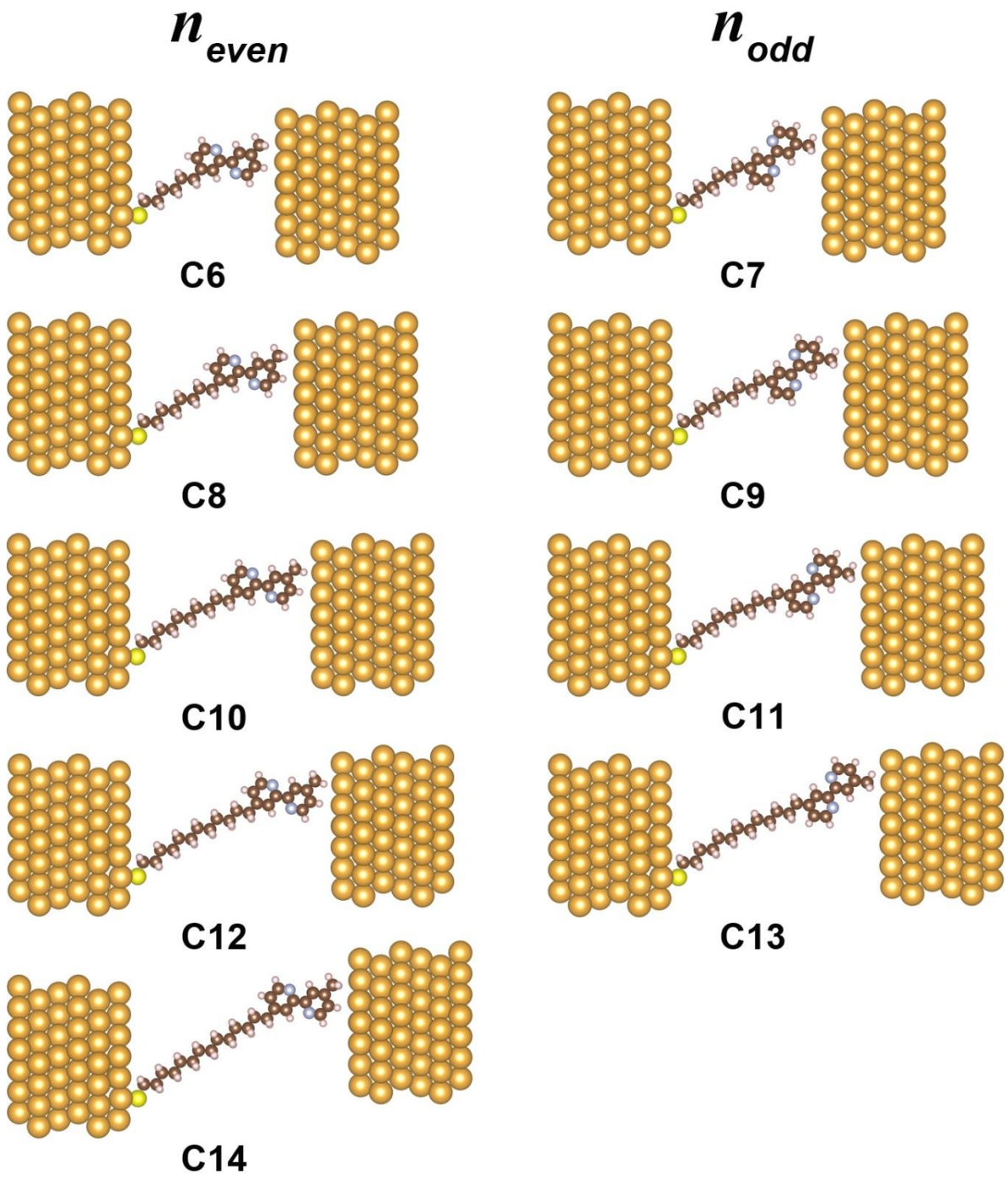

Fig. S1 Schematic illustrations of the central region for all investigated C*n* single-molecule diodes.

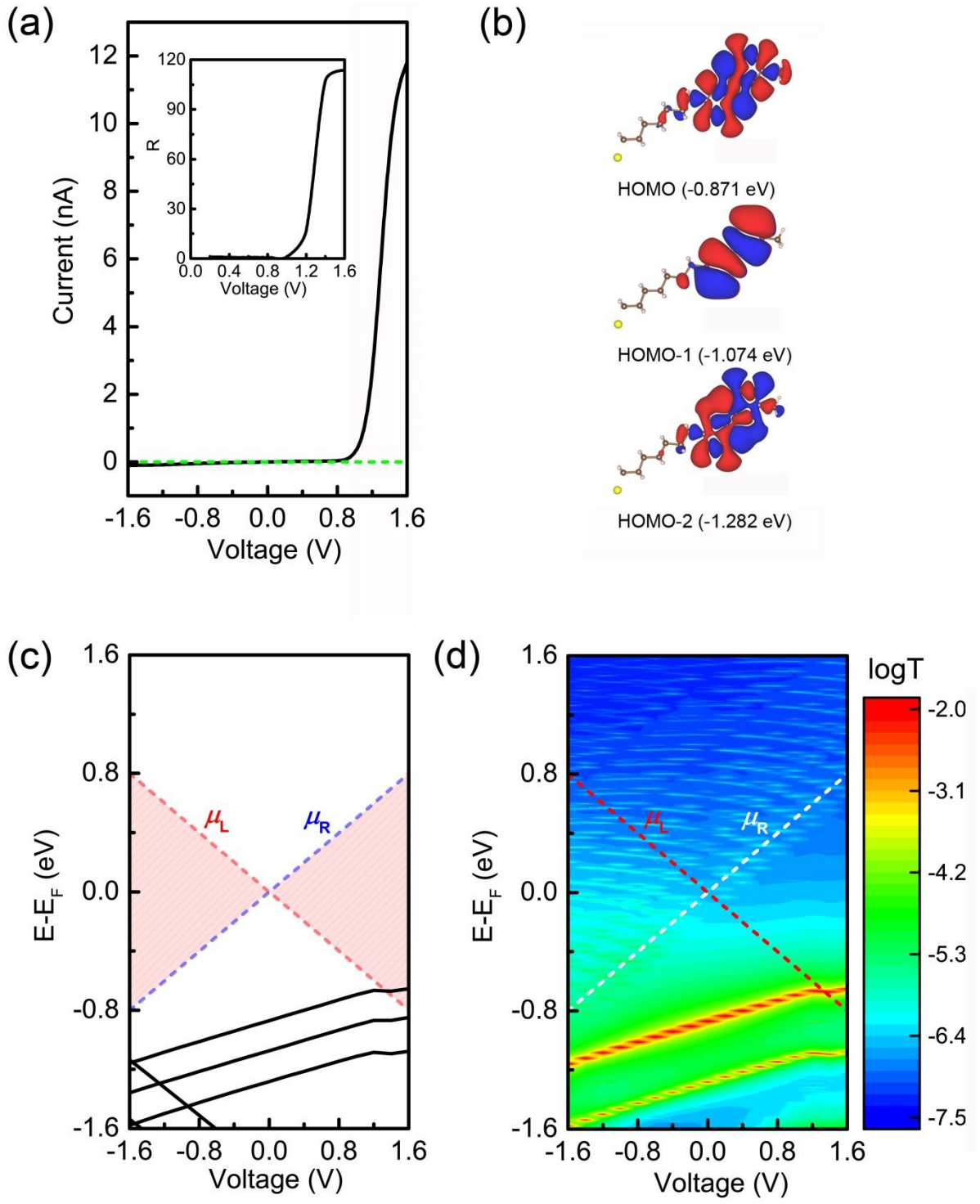

Fig. S2 (a) The current-voltage curve as well as the bias-dependent rectification ratio *R*, (b) spatial distributions of HOMO, HOMO-1, and HOMO-2 at zero bias, (c) energy evolution of frontier molecular orbitals, and (d) electronic transmission spectra for C7. The dashed lines in (c) and (d) show the chemical potential of each electrode. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

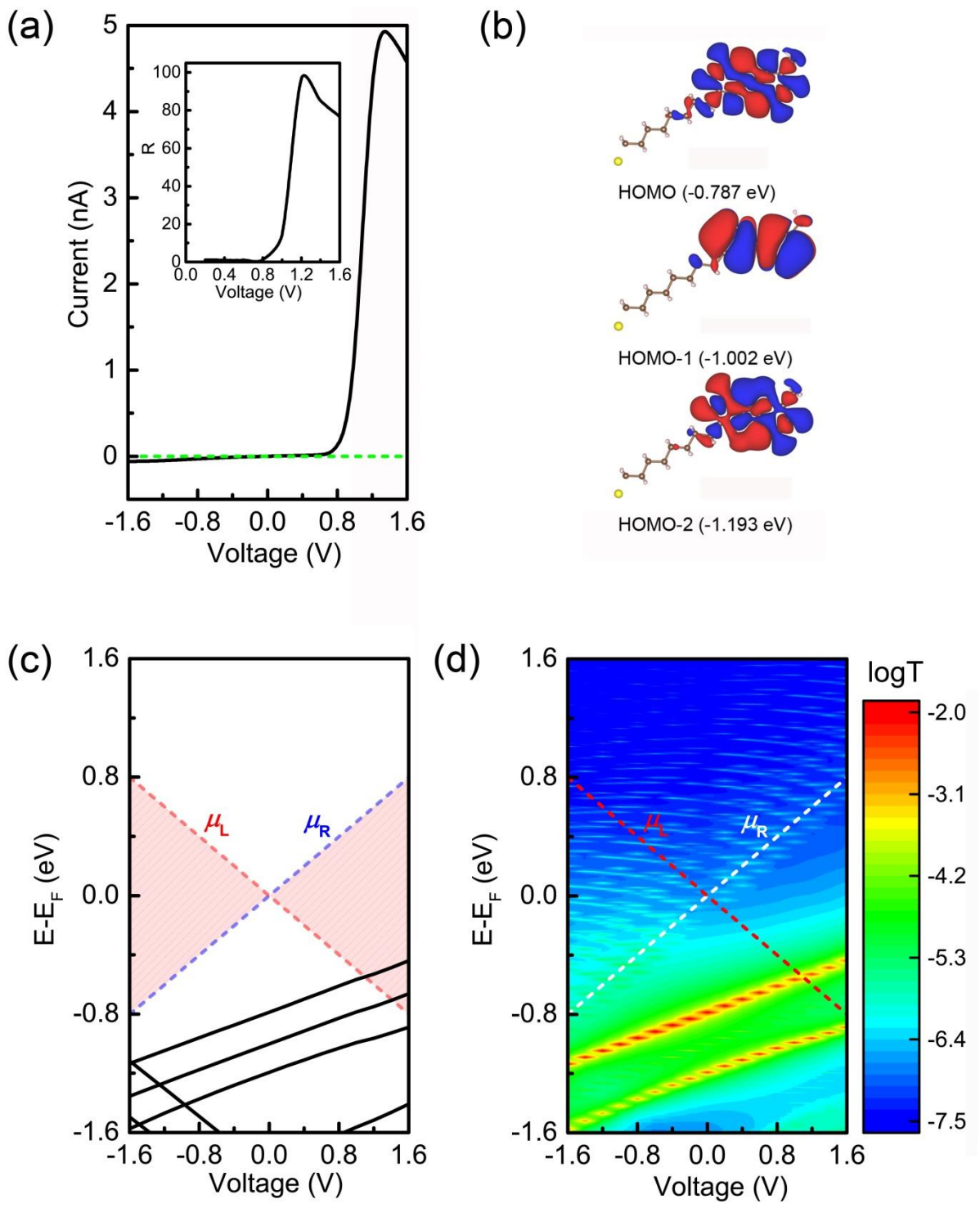

Fig. S3 (a) The current-voltage curve as well as the bias-dependent rectification ratio *R*, (b) spatial distributions of HOMO, HOMO-1, and HOMO-2 at zero bias, (c) energy evolution of frontier molecular orbitals, and (d) electronic transmission spectra for C8. The dashed lines in (c) and (d) show the chemical potential of each electrode. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

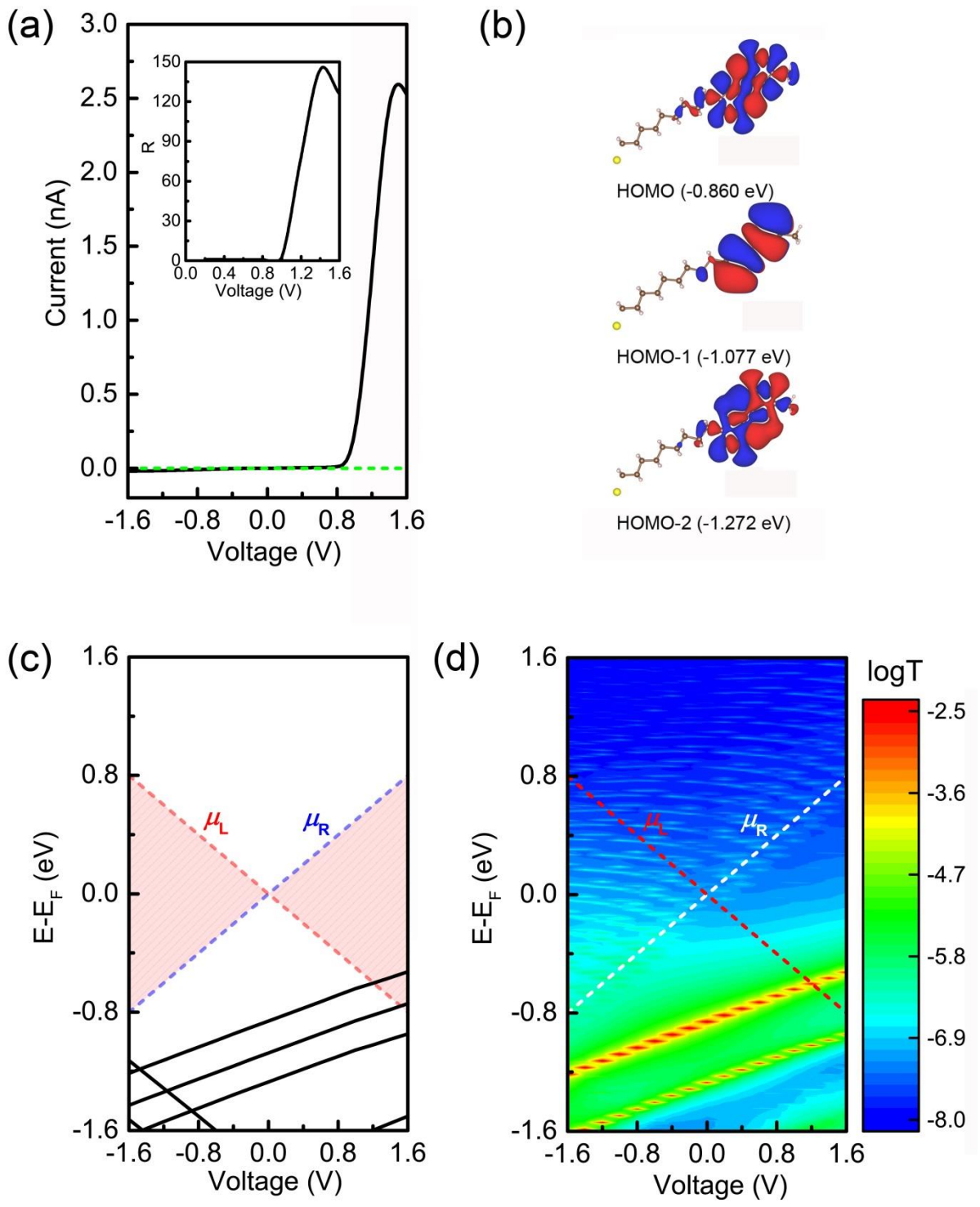

Fig. S4 (a) The current-voltage curve as well as the bias-dependent rectification ratio *R*, (b) spatial distributions of HOMO, HOMO-1, and HOMO-2 at zero bias, (c) energy evolution of frontier molecular orbitals, and (d) electronic transmission spectra for C9. The dashed lines in (c) and (d) show the chemical potential of each electrode. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

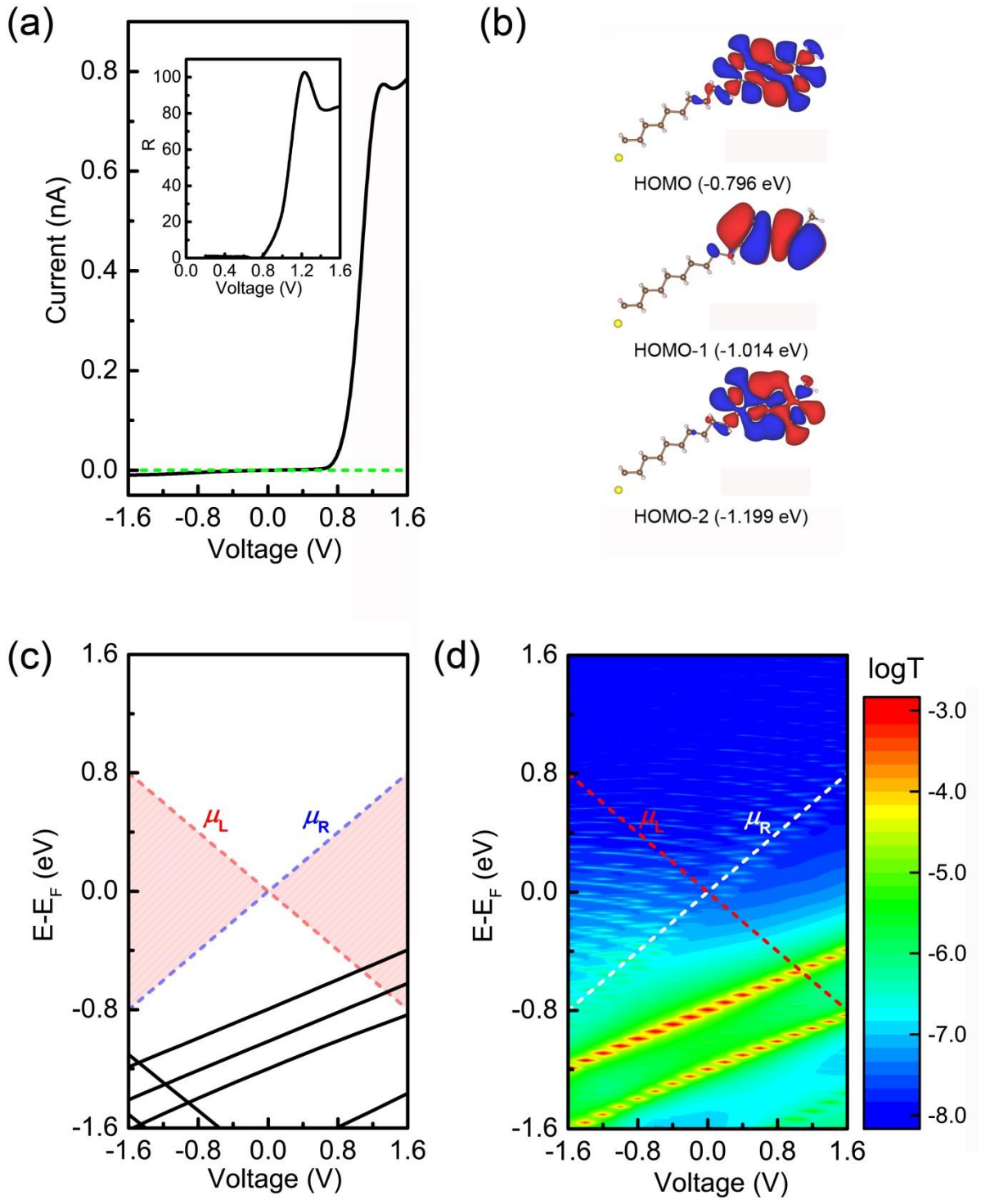

Fig. S5 (a) The current-voltage curve as well as the bias-dependent rectification ratio *R*, (b) spatial distributions of HOMO, HOMO-1, and HOMO-2 at zero bias, (c) energy evolution of frontier molecular orbitals, and (d) electronic transmission spectra for C10. The dashed lines in (c) and (d) show the chemical potential of each electrode. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005. (a) and (d) are taken from Fig. 3(a) and Fig. 3(b), respectively.

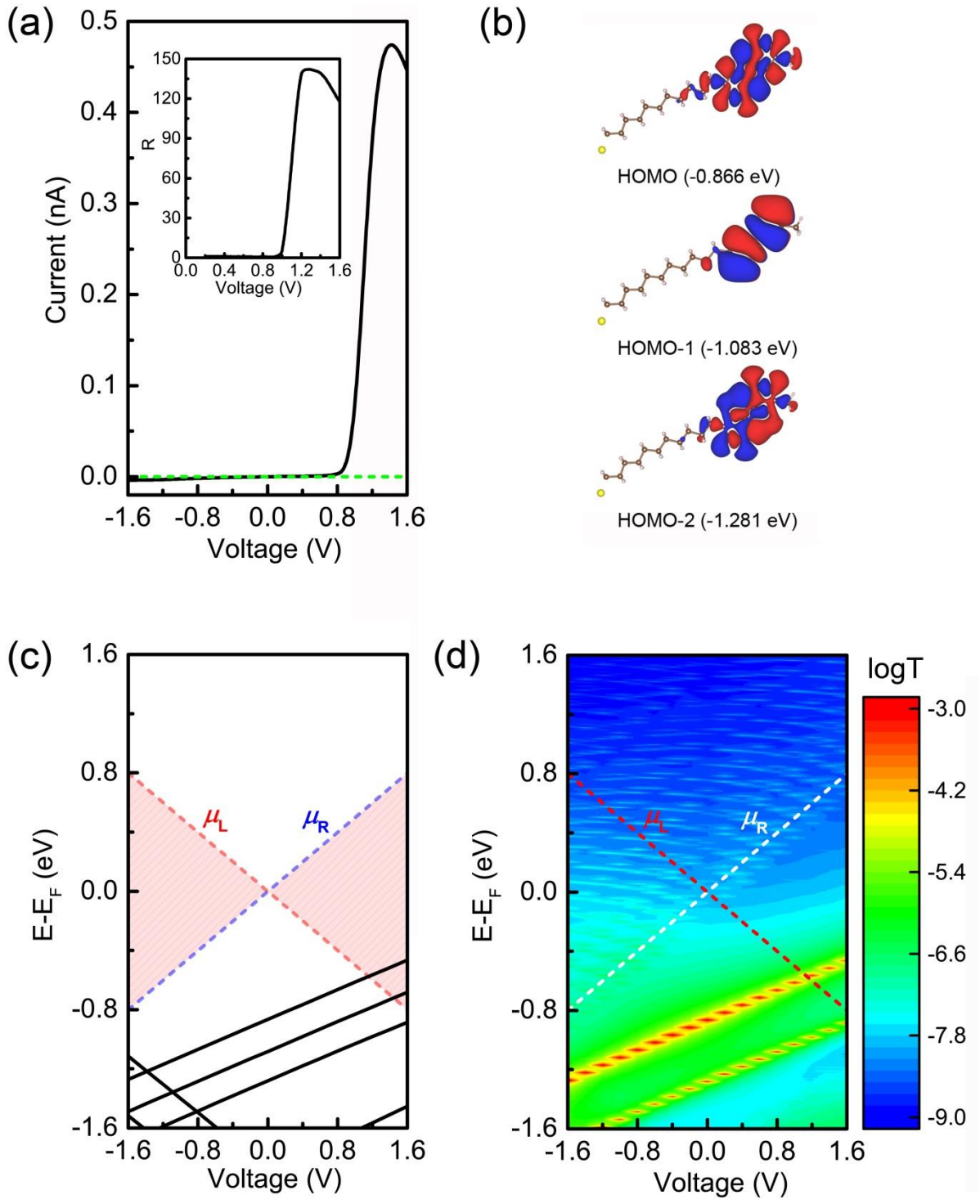

Fig. S6 (a) The current-voltage curve as well as the bias-dependent rectification ratio *R*, (b) spatial distributions of HOMO, HOMO-1, and HOMO-2 at zero bias, (c) energy evolution of frontier molecular orbitals, and (d) electronic transmission spectra for C11. The dashed lines in (c) and (d) show the chemical potential of each electrode. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

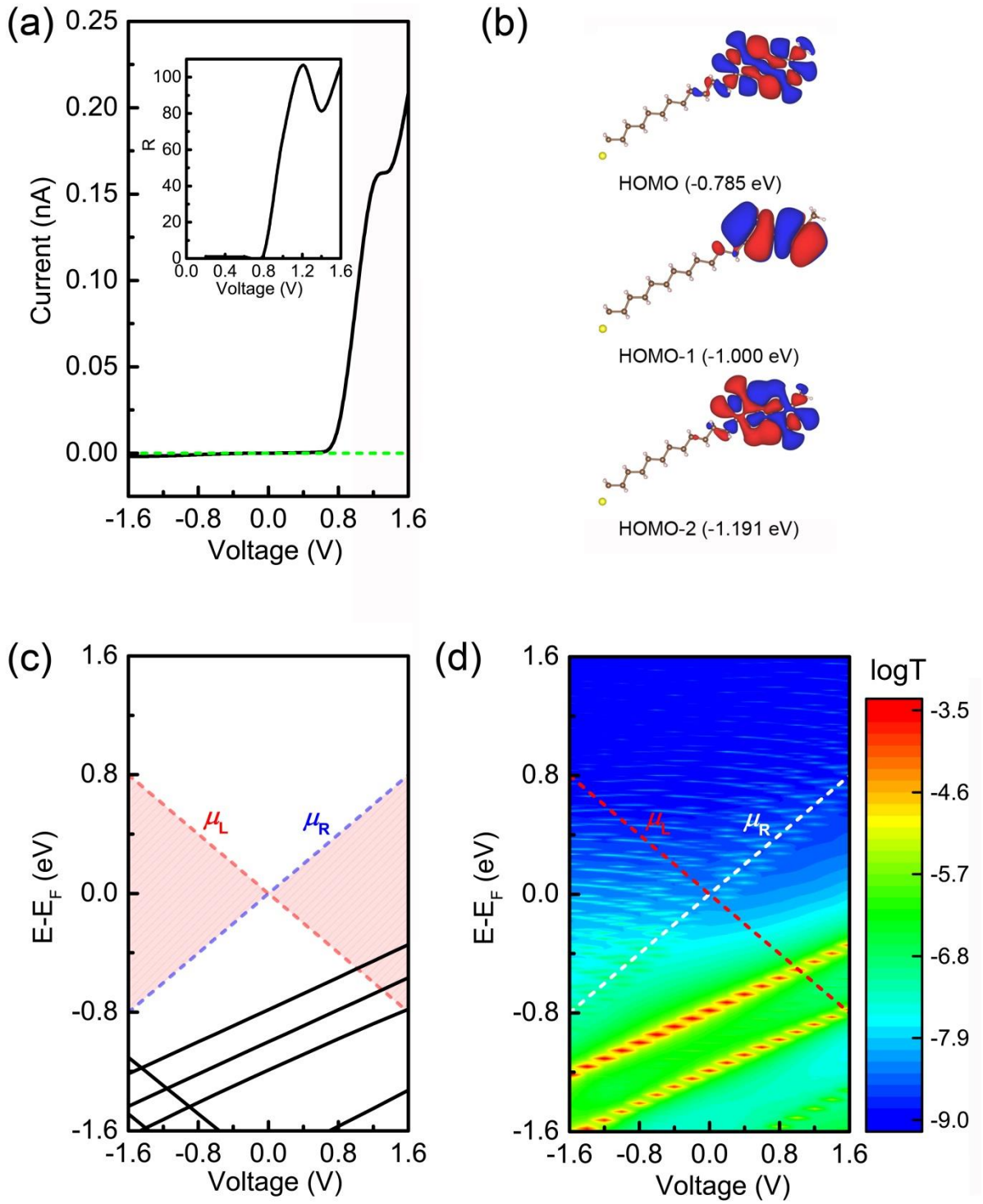

Fig. S7 (a) The current-voltage curve as well as the bias-dependent rectification ratio *R*, (b) spatial distributions of HOMO, HOMO-1, and HOMO-2 at zero bias, (c) energy evolution of frontier molecular orbitals, and (d) electronic transmission spectra for C12. The dashed lines in (c) and (d) show the chemical potential of each electrode. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

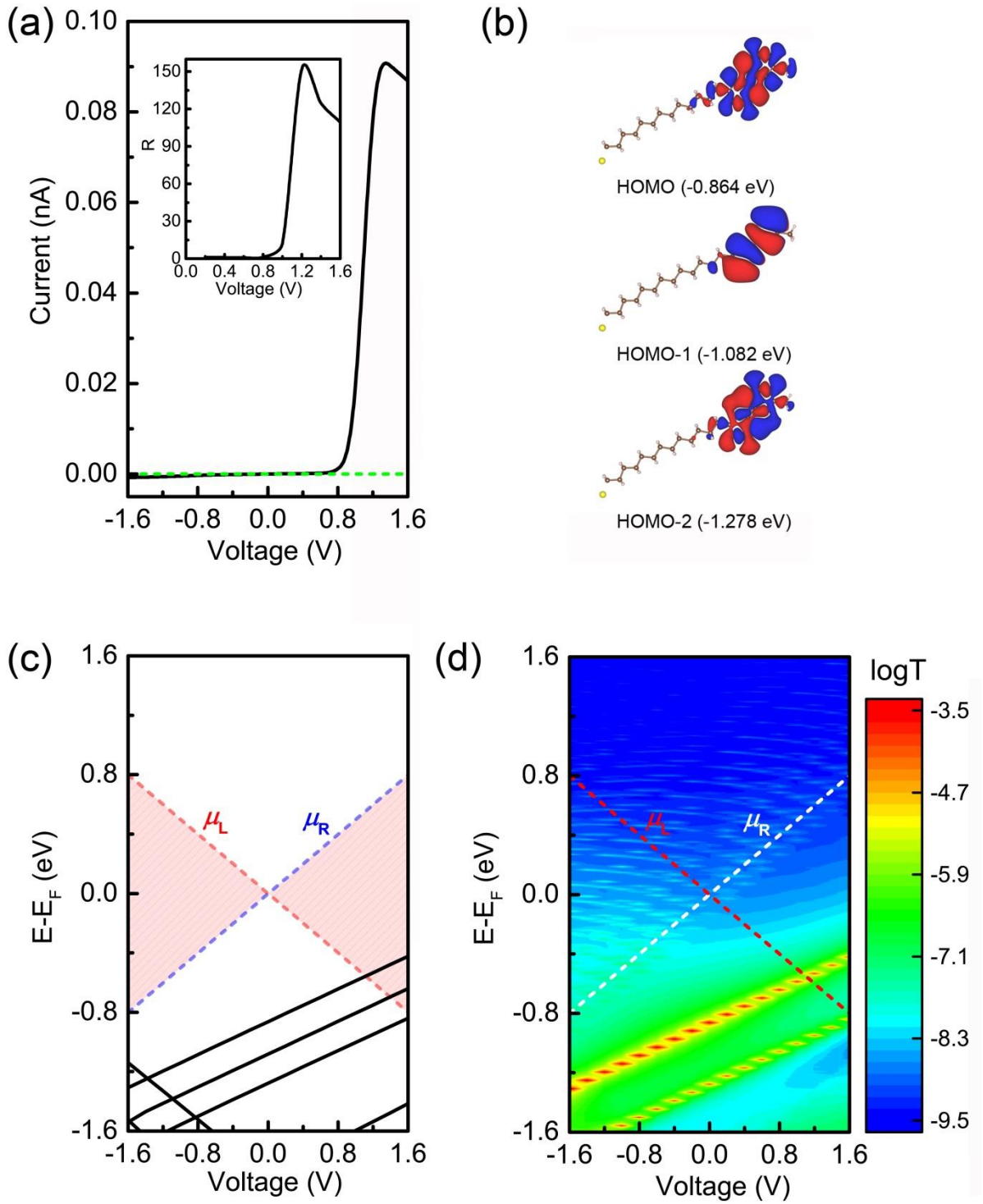

Fig. S8 (a) The current-voltage curve as well as the bias-dependent rectification ratio *R*, (b) spatial distributions of HOMO, HOMO-1, and HOMO-2 at zero bias, (c) energy evolution of frontier molecular orbitals, and (d) electronic transmission spectra for C13. The dashed lines in (c) and (d) show the chemical potential of each electrode. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

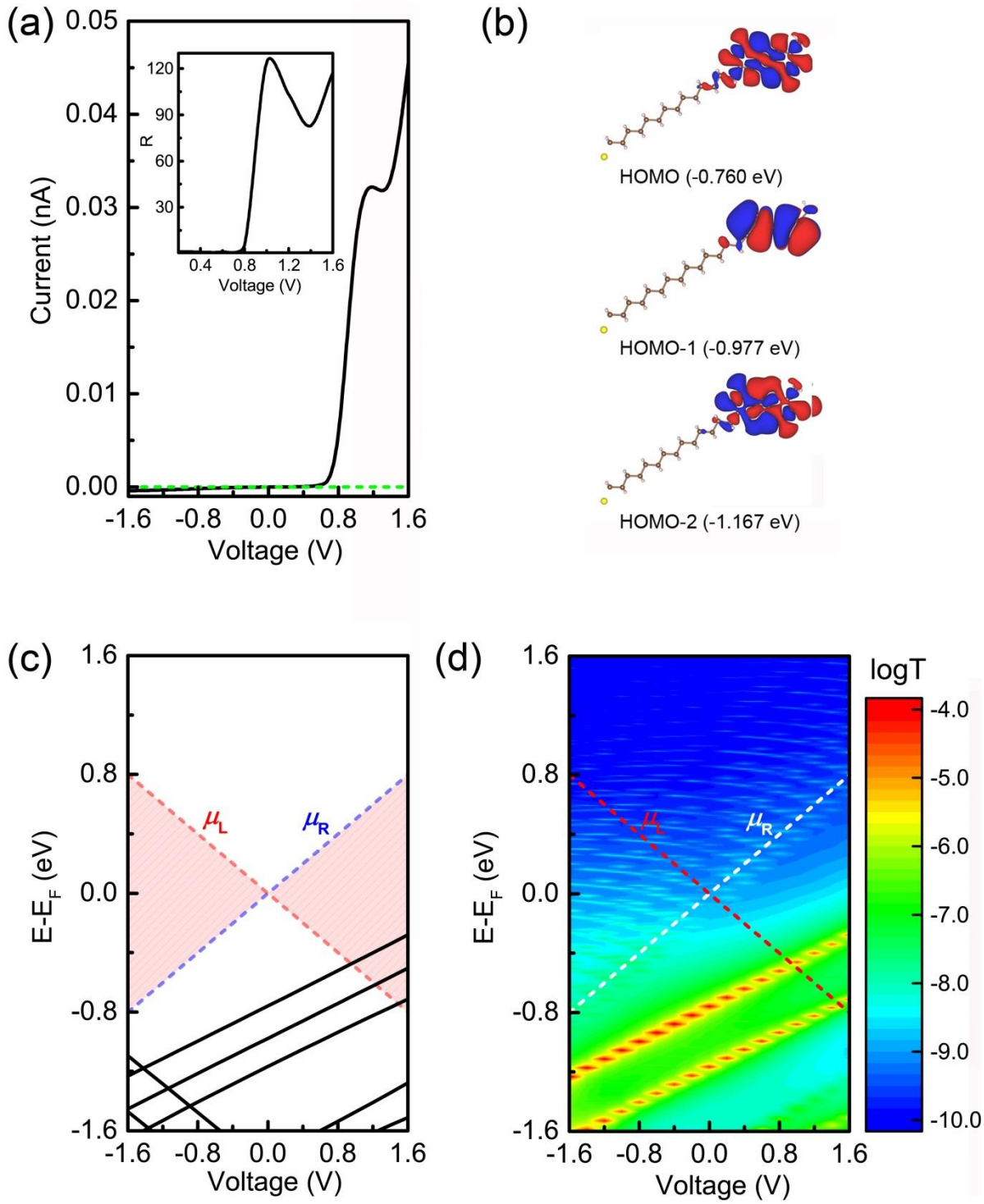

Fig. S9 (a) The current-voltage curve as well as the bias-dependent rectification ratio *R*, (b) spatial distributions of HOMO, HOMO-1, and HOMO-2 at zero bias, (c) energy evolution of frontier molecular orbitals, and (d) electronic transmission spectra for C14. The dashed lines in (c) and (d) show the chemical potential of each electrode. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005. (a) and (d) are taken from Fig. 3(c) and Fig. 3(d), respectively.

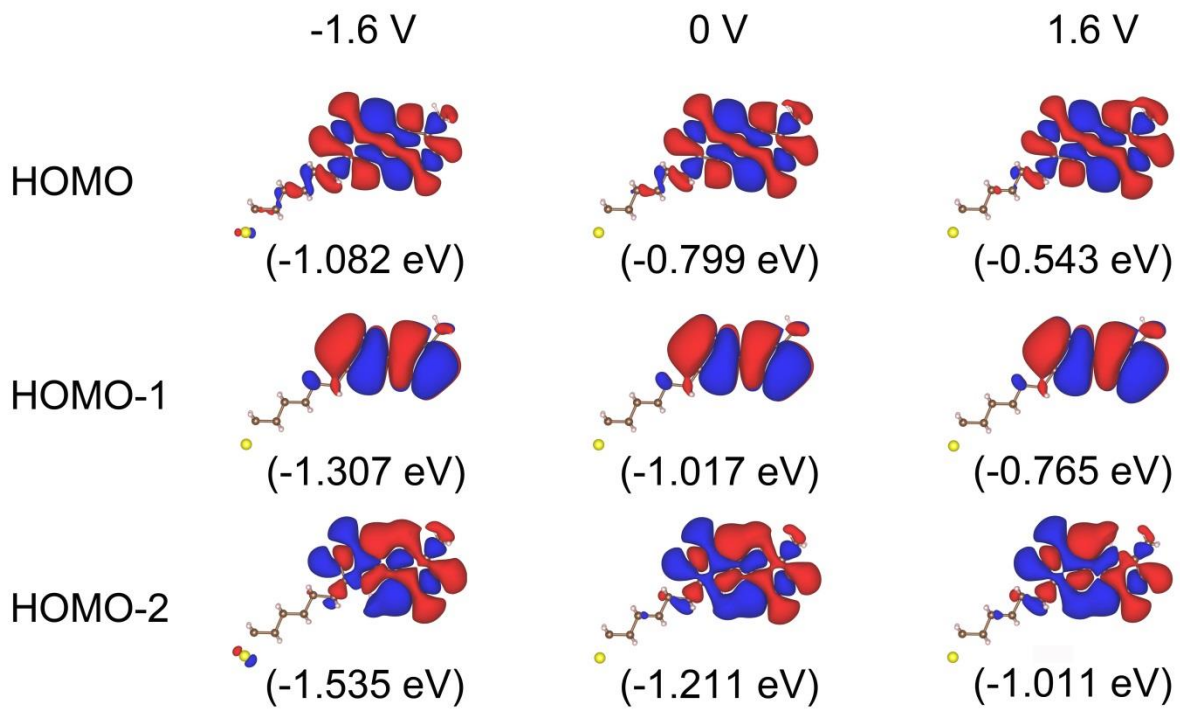

Fig. S10 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C6 single-molecule diode. Those at 0 V are taken from Fig. 2(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

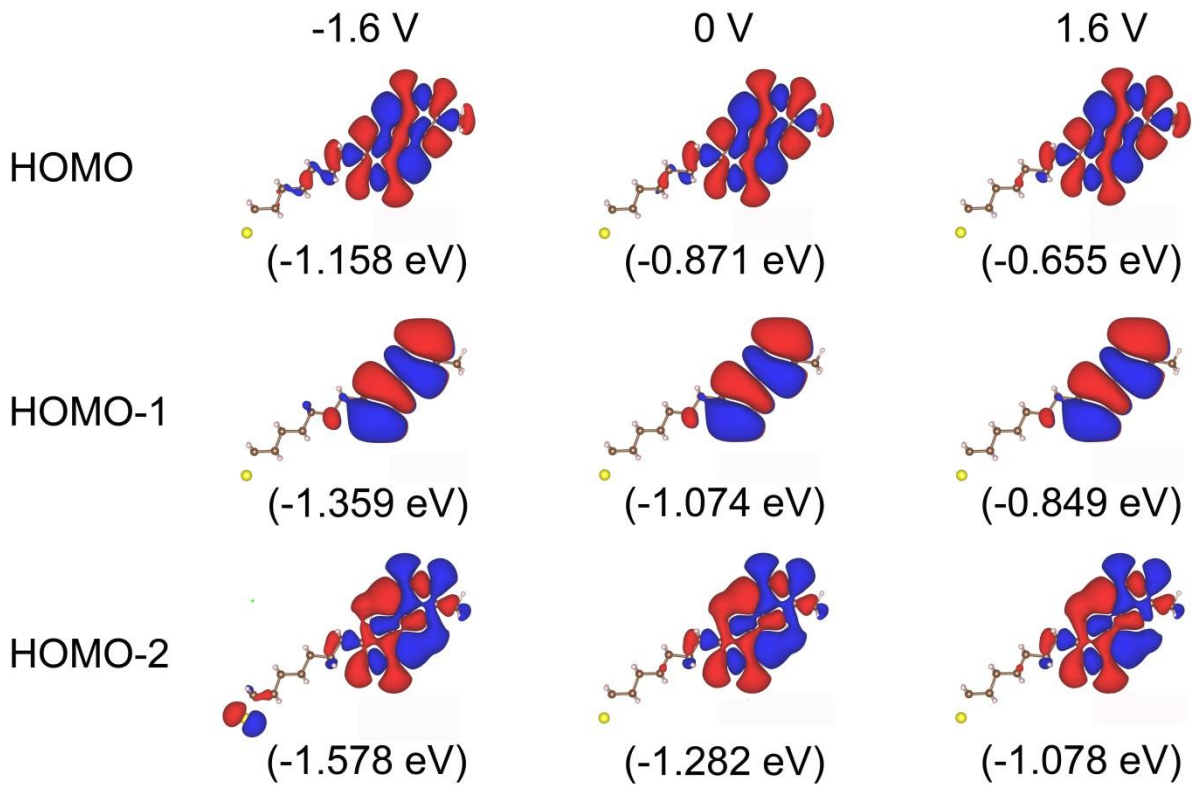

Fig. S11 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C7 single-molecule diode. Those at 0 V are taken from Fig. S2(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

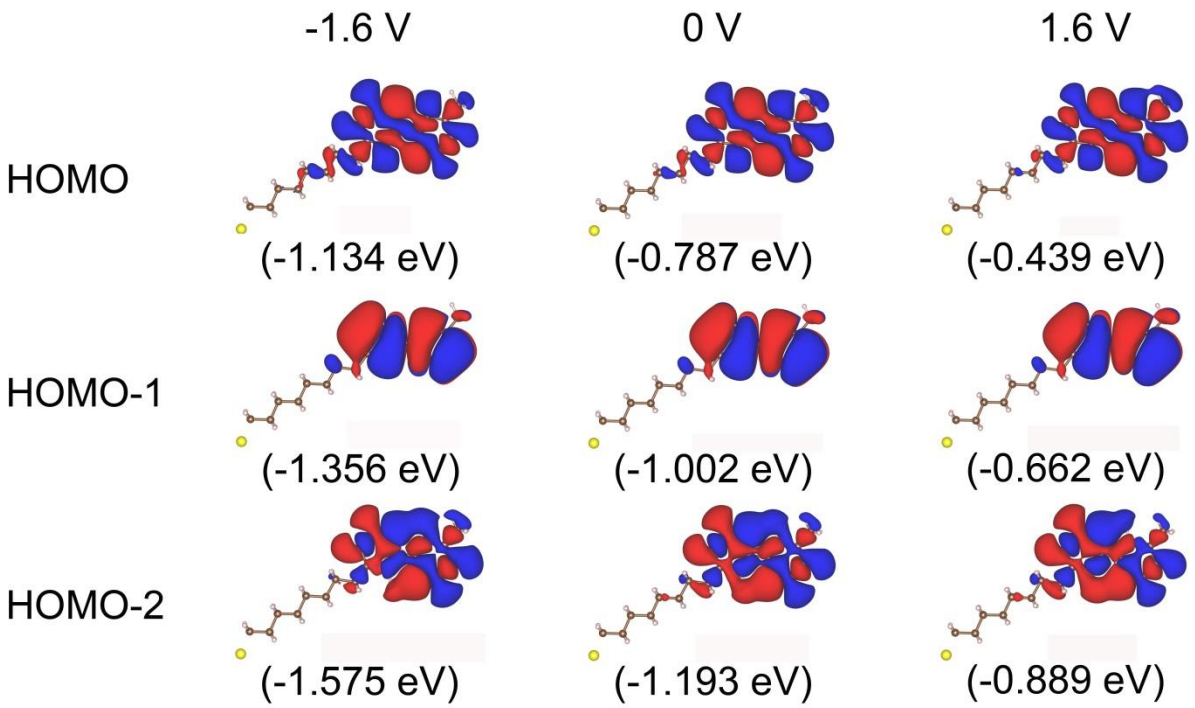

Fig. S12 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C8 single-molecule diode. Those at 0 V are taken from Fig. S3(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

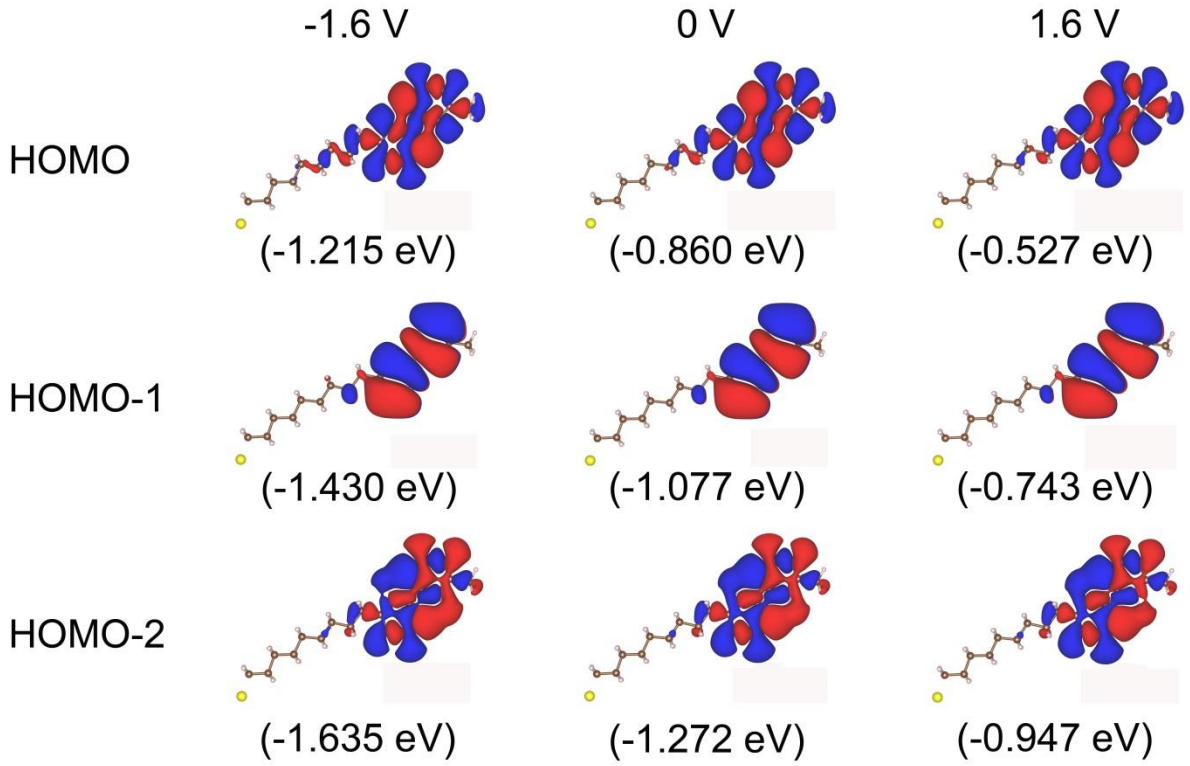

Fig. S13 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C9 single-molecule diode. Those at 0 V are taken from Fig. S4(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

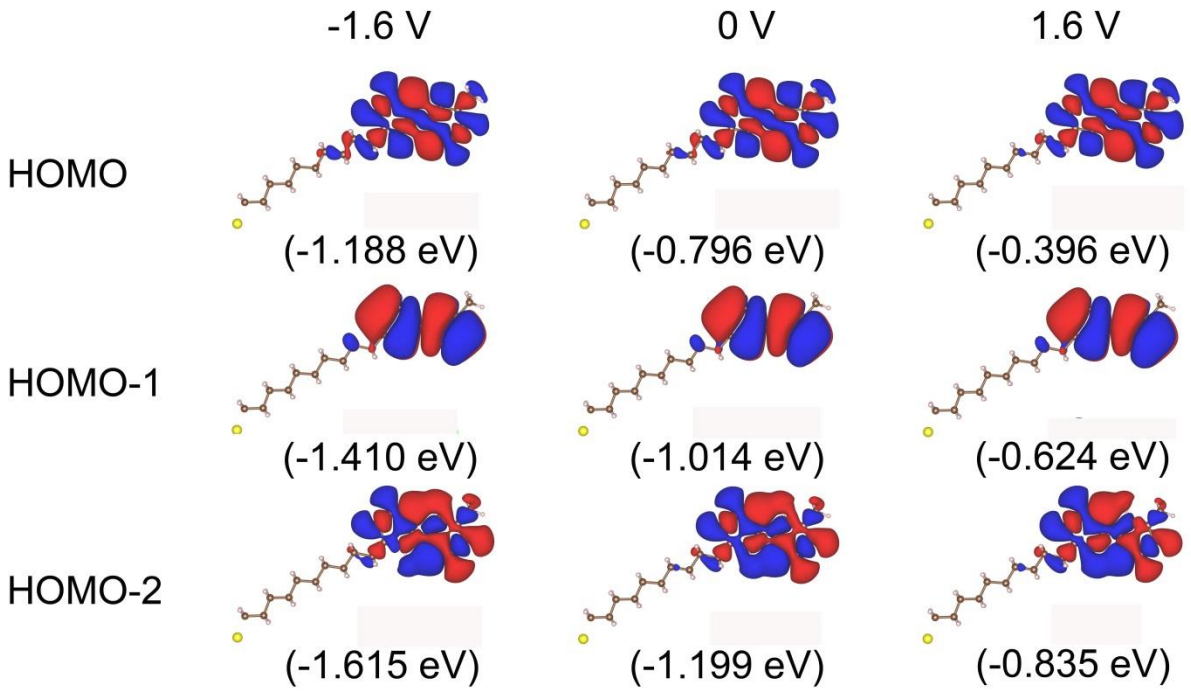

Fig. S14 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C10 single-molecule diode. Those at 0 V are taken from Fig. S5(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

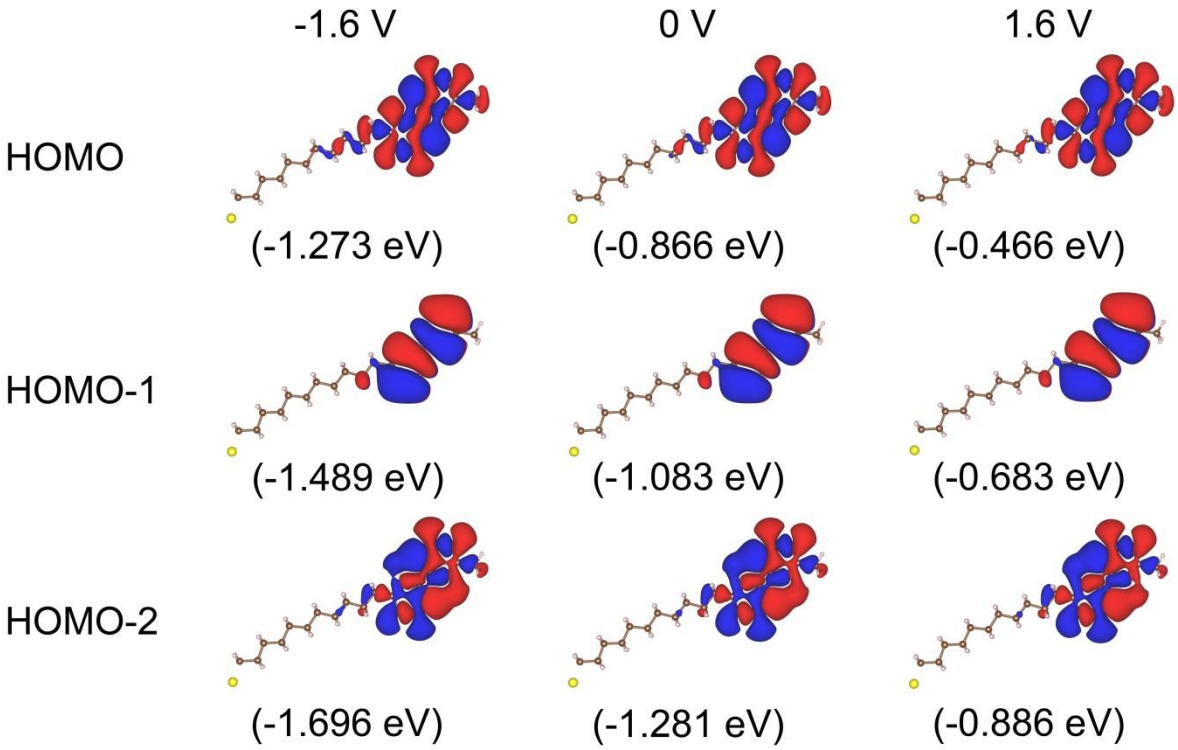

Fig. S15 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C11 single-molecule diode. Those at 0 V are taken from Fig. S6(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

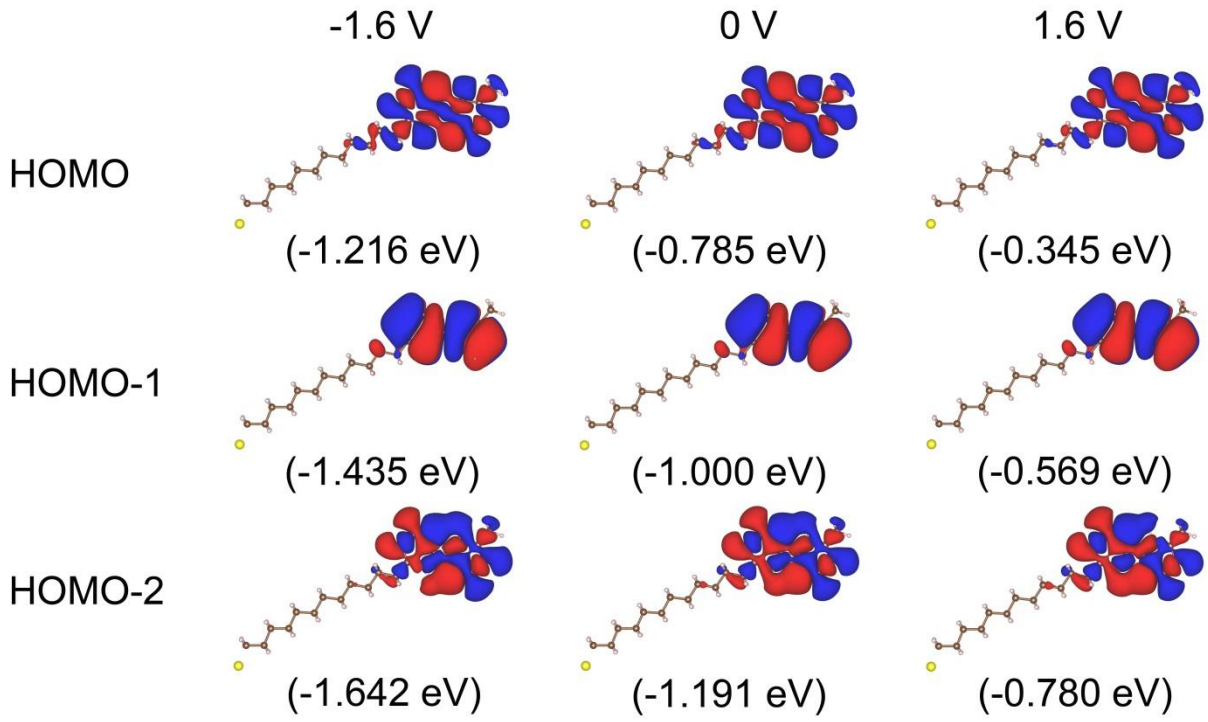

Fig. S16 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C12 single-molecule diode. Those at 0 V are taken from Fig. S7(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

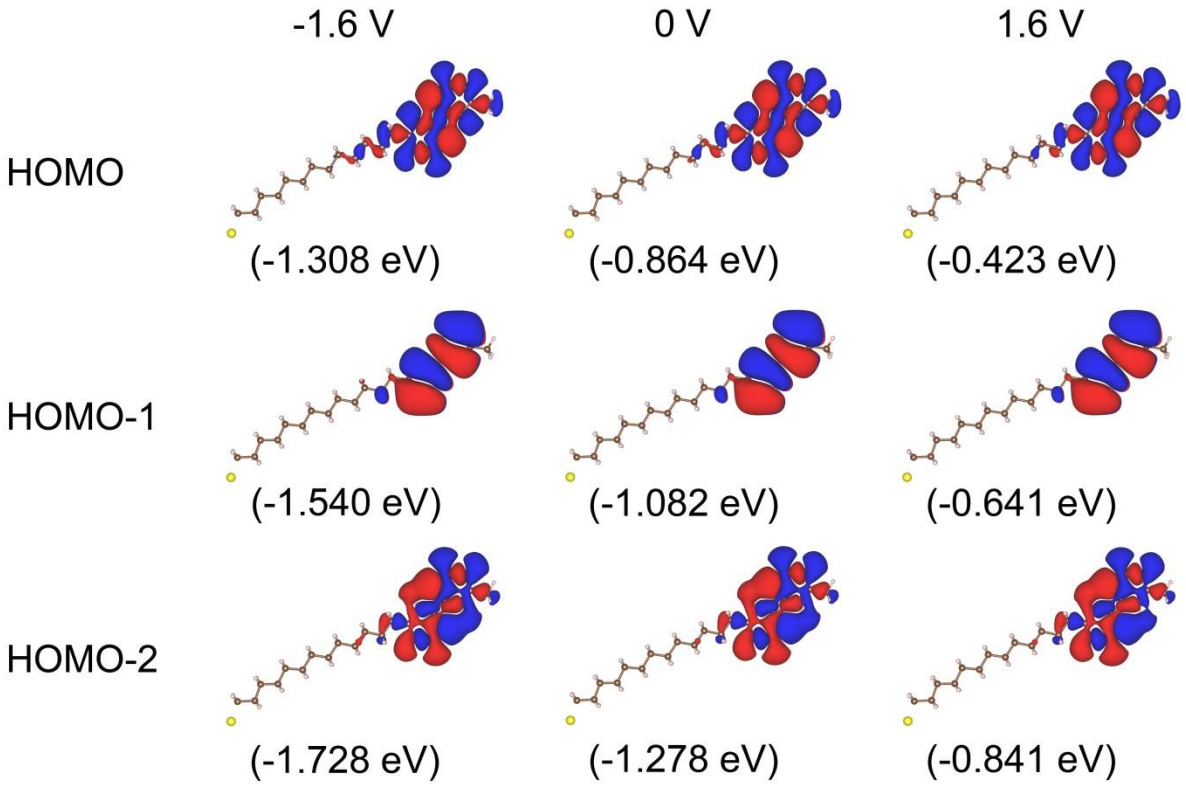

Fig. S17 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C13 single-molecule diode. Those at 0 V are taken from Fig. S8(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.

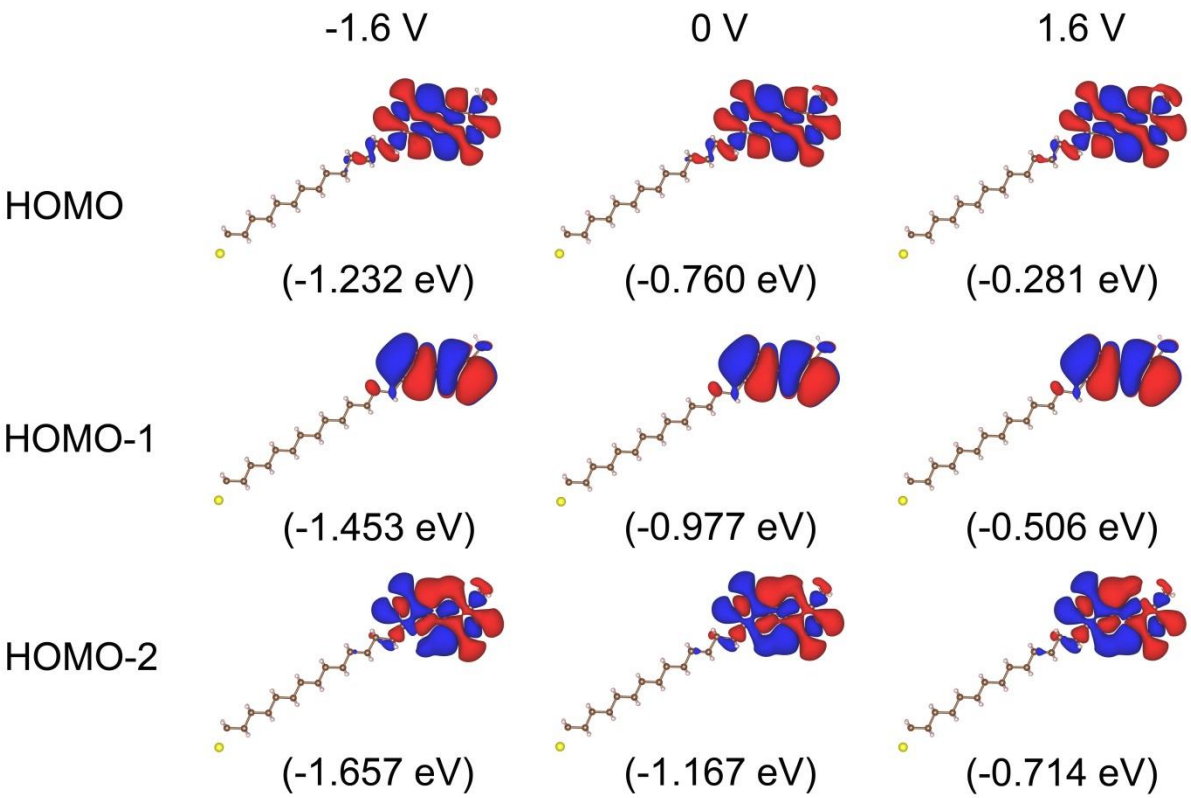

Fig. S18 Spatial distributions of HOMO, HOMO-1, and HOMO-2 under 0 V, ±1.6 V for C14 single-molecule diode. Those at 0 V are taken from Fig. S9(b) for an easy comparison. The isovalue for displaying wavefunctions of frontier molecular orbitals is 0.005.