Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Silver electrodes provide higher conductance than gold for thiol-terminated oligosilane molecular junctions: the interfacial effect

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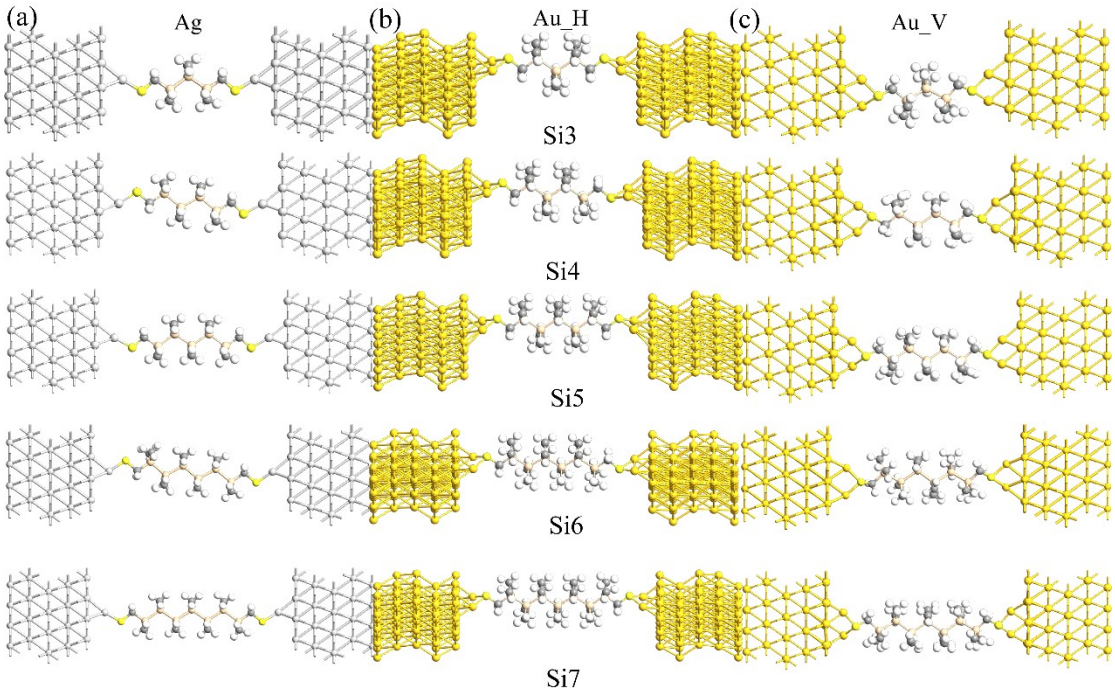

Fig. S1 Optimized geometric structures of molecular junctions for Si3–Si7 with different electrode materials and interfacial configurations. (a) Ag (111) with one protruding Ag atom surface; (b,c) Au(111) electrode with the vertical/horizontal configuration of a double atomic surface (Au_V/Au_H).

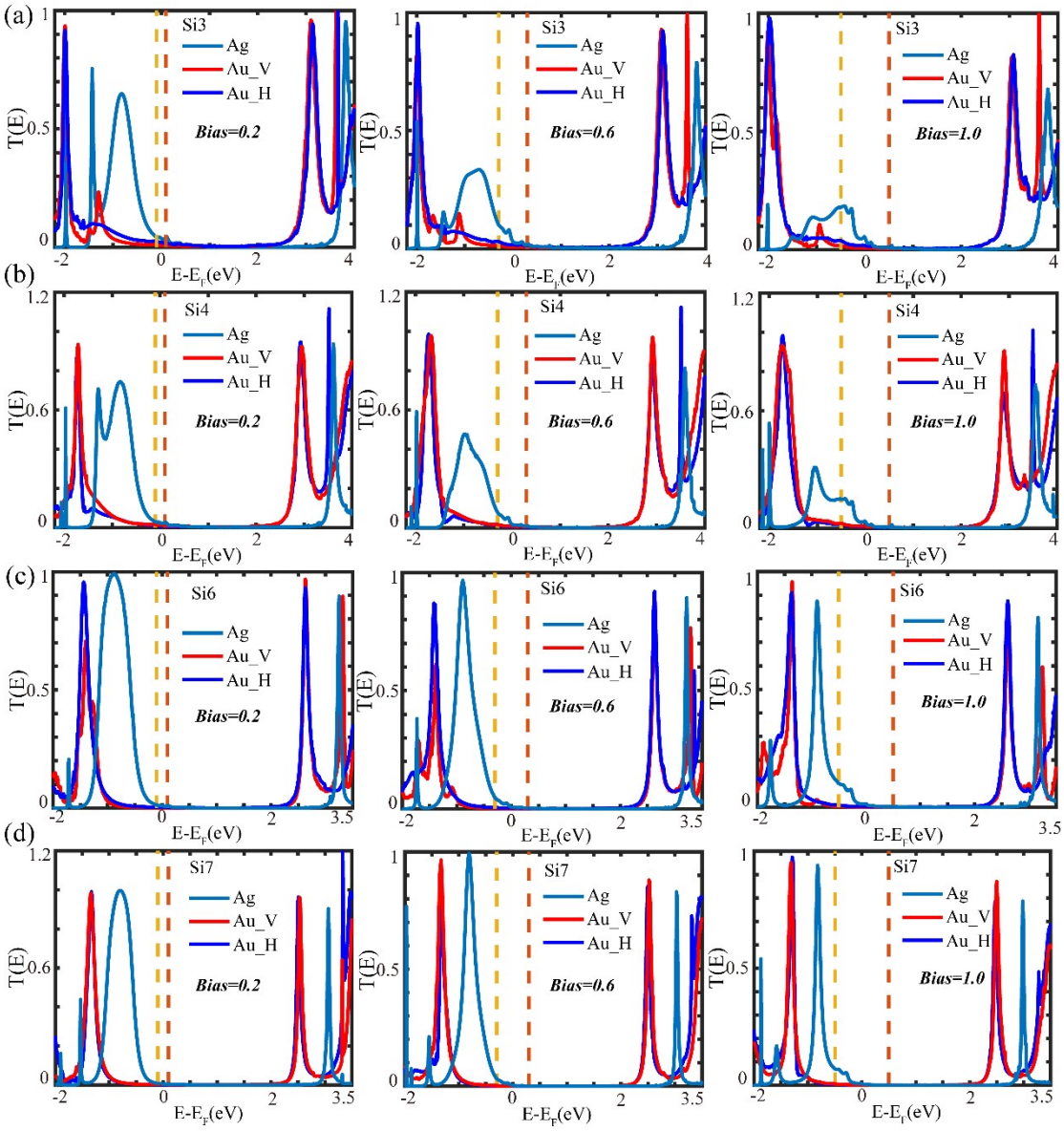

Fig. S2 Transmission spectra calculated at different applied bias voltages of 0.2, 0.6, and 1.0 V for (a) Si3, (b) Si4, (c) Si6, and (d) Si7.

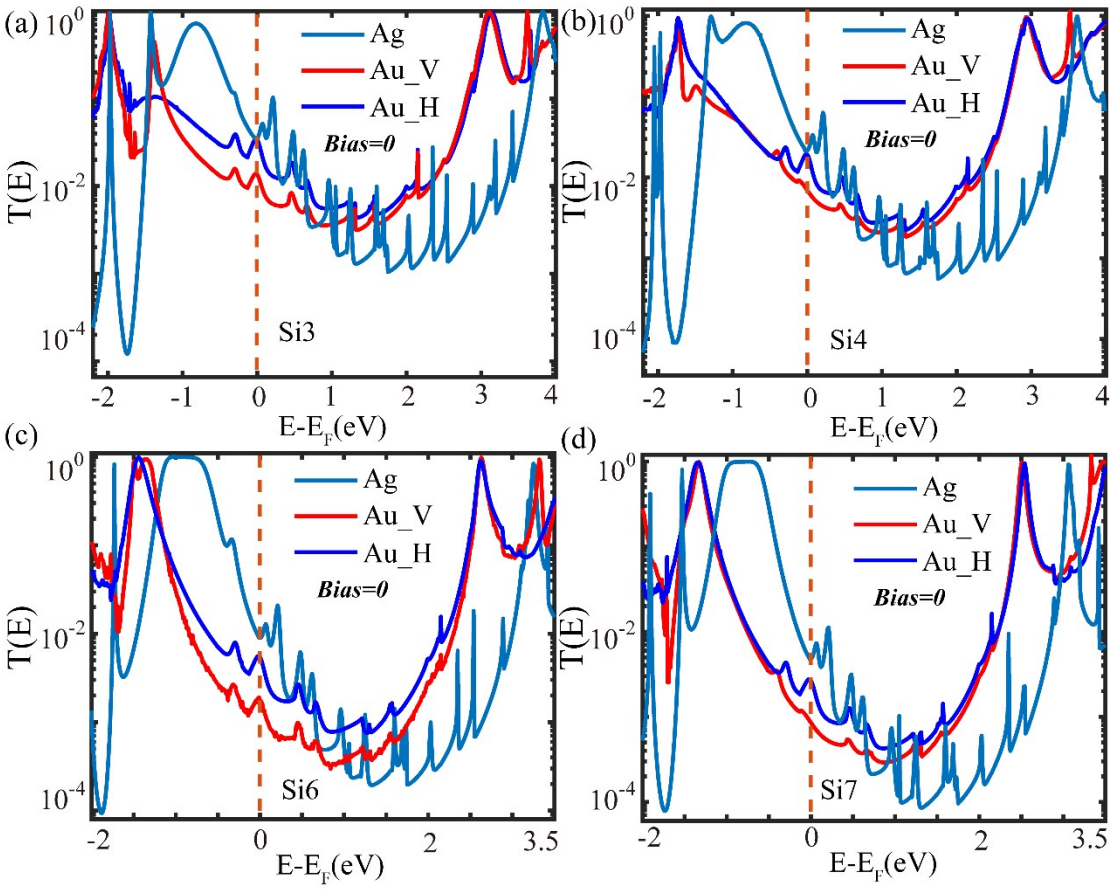

Fig. S3 Equilibrium transmission spectra of the (a) Si3, (b) Si4, (c) Si6, and (d) Si7 molecular junctions with electrodes and interfaces denoted as Ag, Au_V, and Au_H.

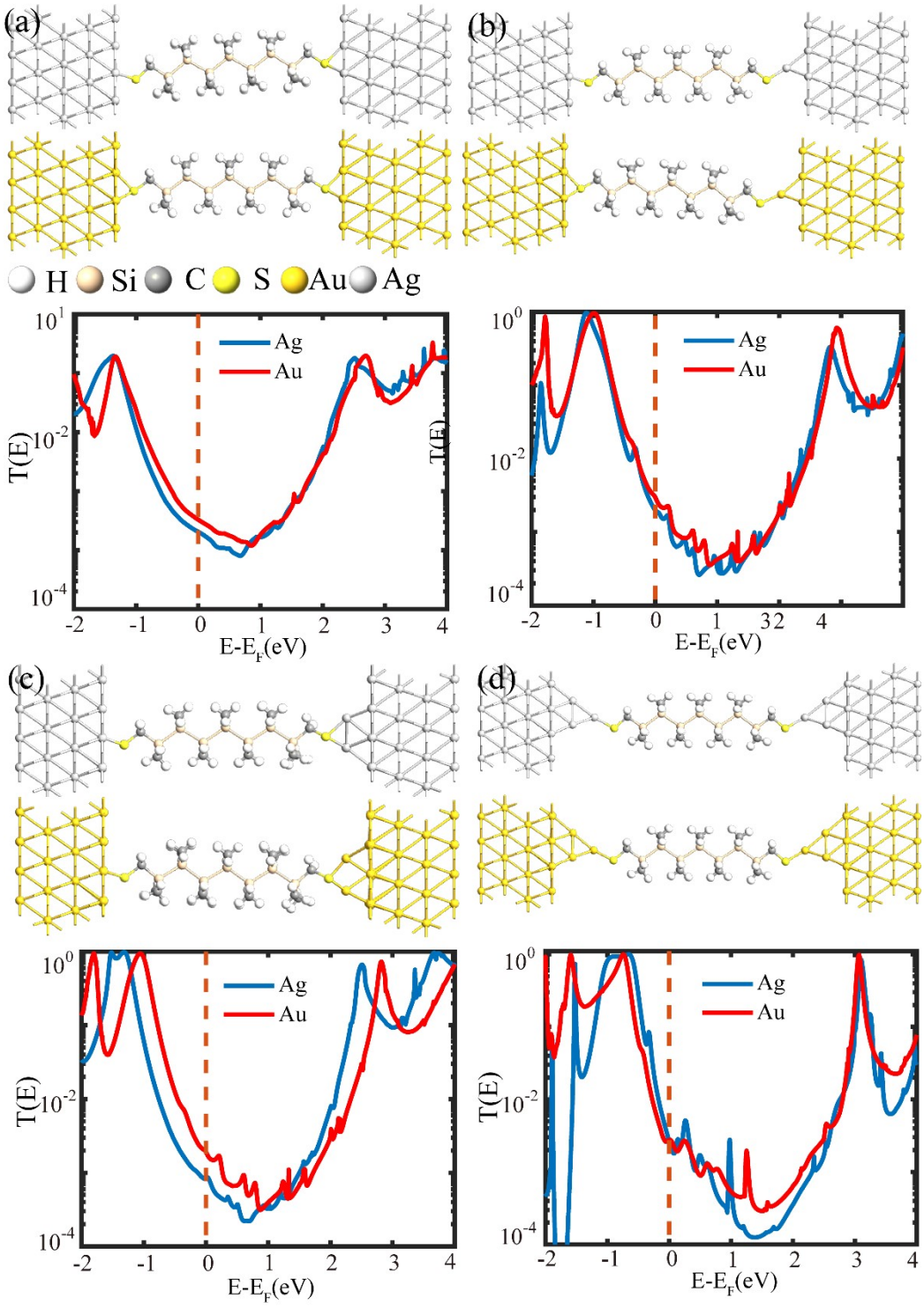

Fig. S4 Optimized molecular junctions and the corresponding transmission curves. (a) The S atoms connected directly to both Ag(111) (top)/Au(111) (bottom) surfaces, (b) the left S atom directly connected to the Ag(111) (top)/Au(111) (bottom) surface and the right S atom connected to a Ag/Au adatom, (c) the left S atom directly connected to the Ag(111) (top)/Au(111) (bottom) surface and the right S atom connected to a double Ag/Au atomic surface with a vertical configuration, and (d) the S atoms connected symmetrically to top-pyramidal Ag/Au atoms. The hydrogen, silicon, carbon, sulfur, gold, and silver atoms are denoted by white, light brown, dark gray, bright yellow, dark yellow, and light gray spheres, respectively.