Electronic Supplementary Material (ESI) for Nanoscale.

Thermoelectric properties of oligoglycine molecular wires

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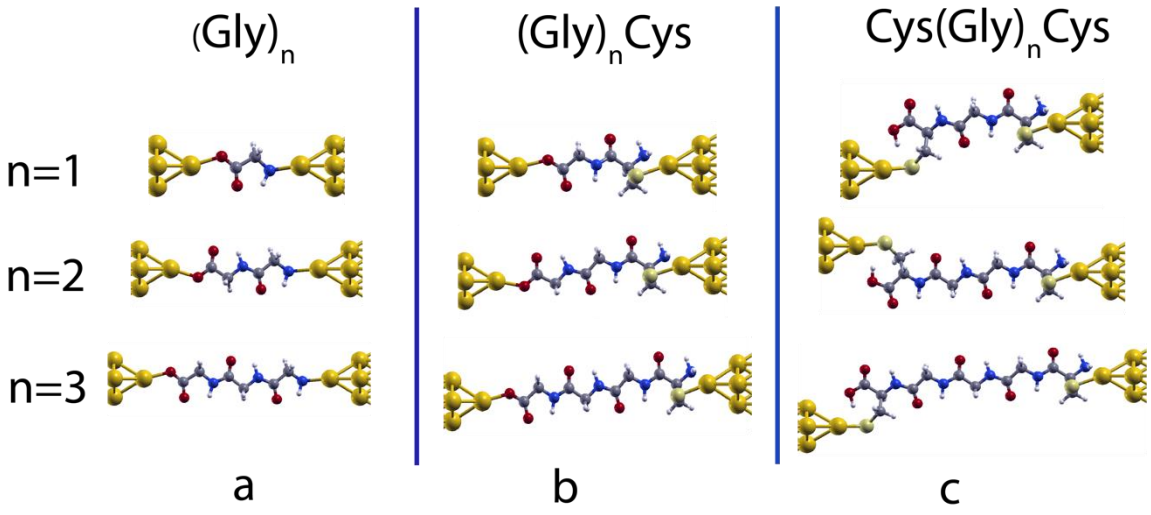


Figure S1. Au-molecule-Au junctions of oligolycine system with three different anchors. The red, grey, white, blue and pale yellow balls represent oxygen, carbon, hydrogen nitrogen and sulphur respectively. Four yellow balls at both ends represent gold leads.

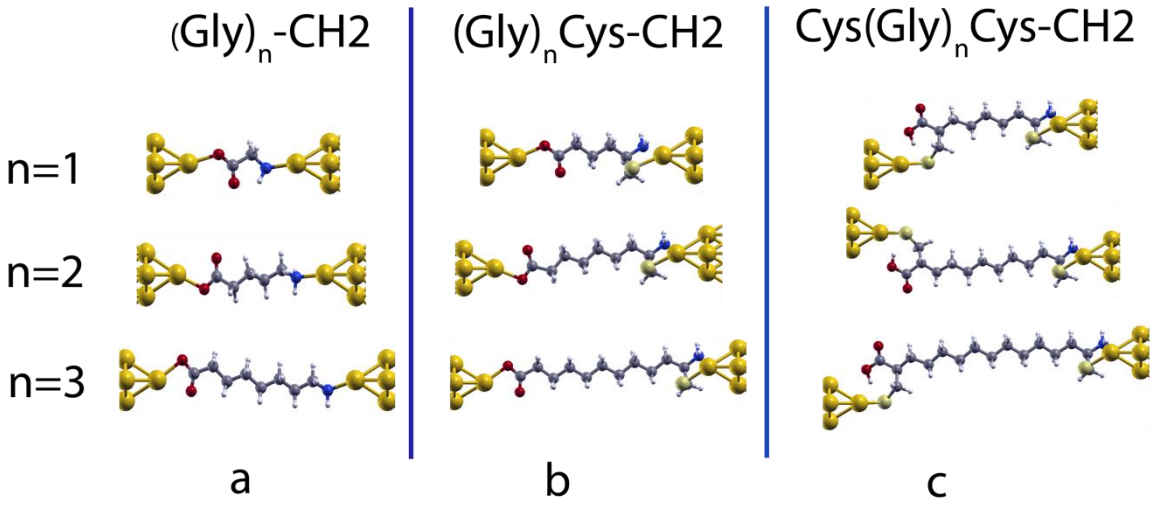


Figure S2. Basing on the structures in figure S1, we replace the peptide bonds in the middle of the molecules without changing the anchors to obtain the β factor.

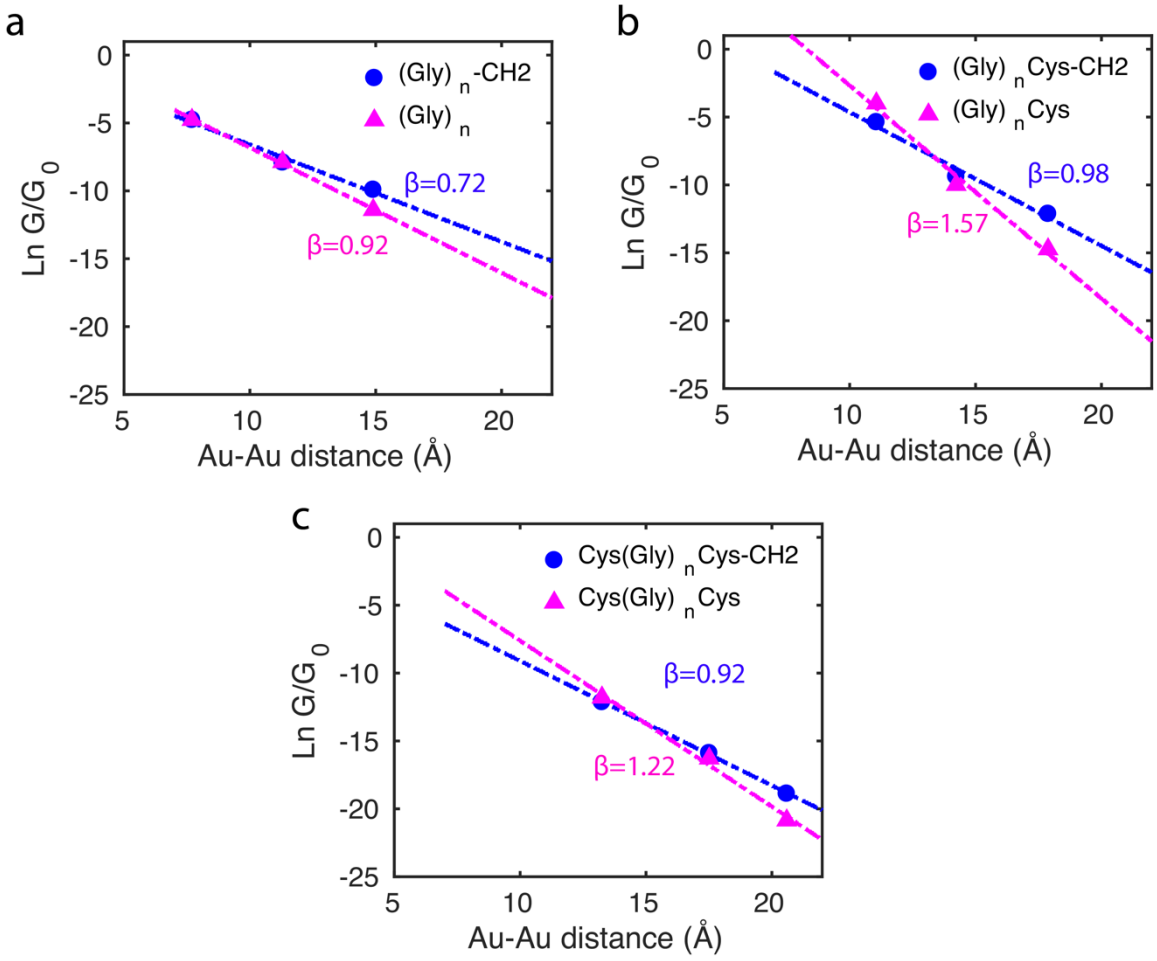
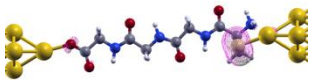
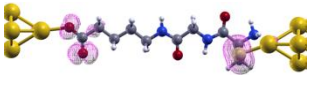
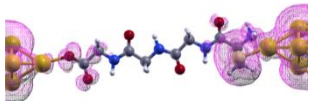
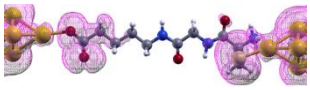
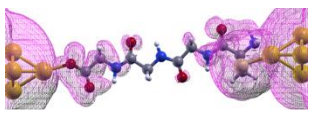
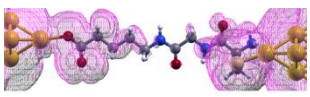
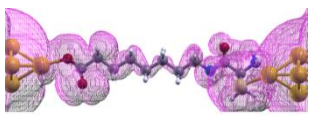


Figure S3. Comparison between β factors of oligoglycine before and after substituting peptide bond with -CH2- corresponding the structures shown in Figure S1 and Figure S2 . (a) $(Gly)_n$, (b) $(Gly)_nCys$ and (c) $Cys(Gly)_nCys$. Which shows after substituting with -CH2- group, the β factor becomes lower for each series comparing with peptide chain.

isosurface	$(Gly)_3Cys$	$(Gly)_3Cys$-A	$(Gly)_3Cys$-B
0.01			
0.001			
0.0001			

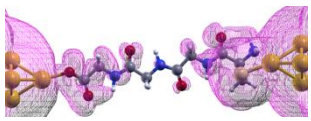
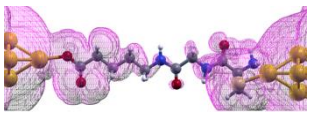
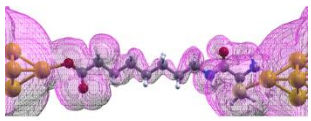
0.00006			

Table S1. The LDOS with magenta color in the energy window from -0.5 to 0 for $(Gly)_3Cys$, $(Gly)_3Cys$-A and $(Gly)_3Cys$-B incorporated in two gold leads separately with the decreasing isosurface from 0.01 to 0.00006.

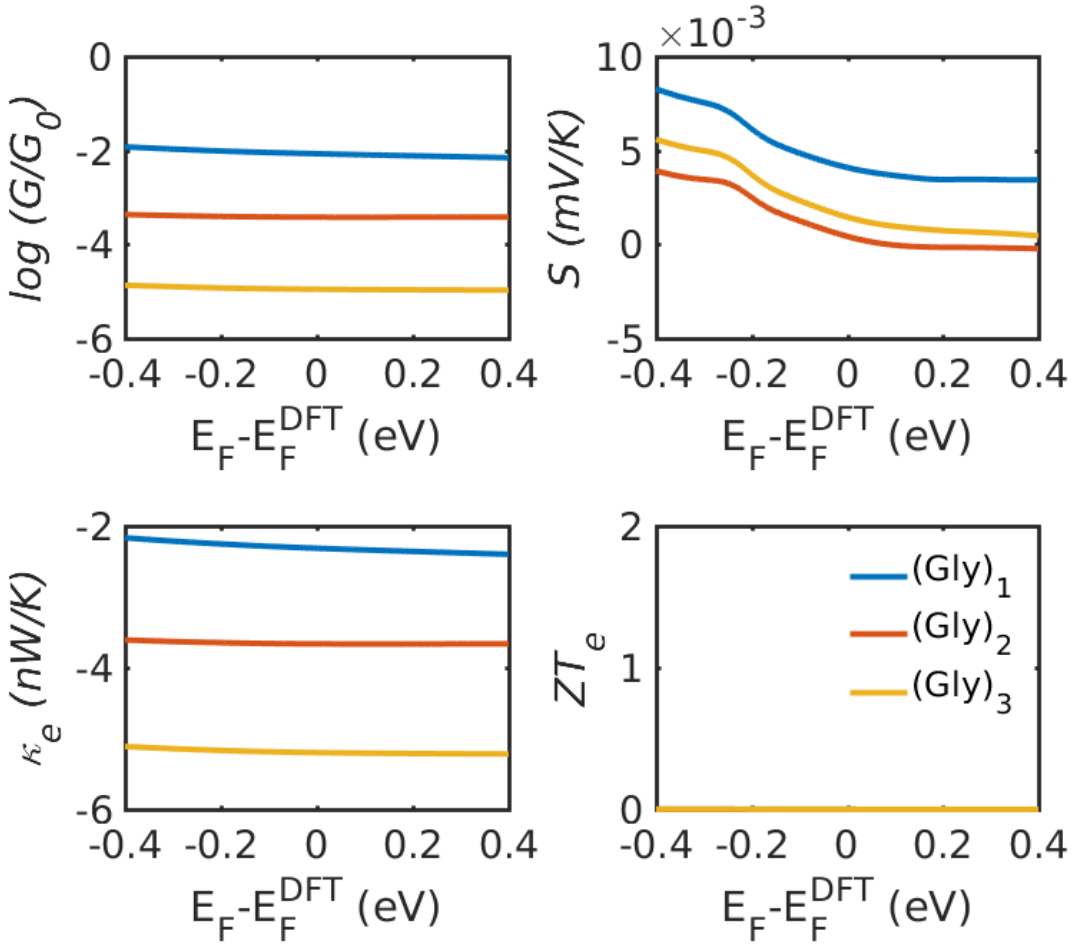


Figure S4. Thermoelectric properties as the function of energy relative to DFT-estimated Fermi energy $E_F - E_F^{DFT}$ at room temperature 300 K for $(Gly)_n$ series. (a) Electrical conductance (G), (b) Seebeck coefficients (S), (c)-(d) Electronic contribution to thermal conductance (κ_e) and figure of merit ZT_e . The blue, red and orange curves represent the Gly, $(Gly)_2$ and $(Gly)_3$ junctions respectively.

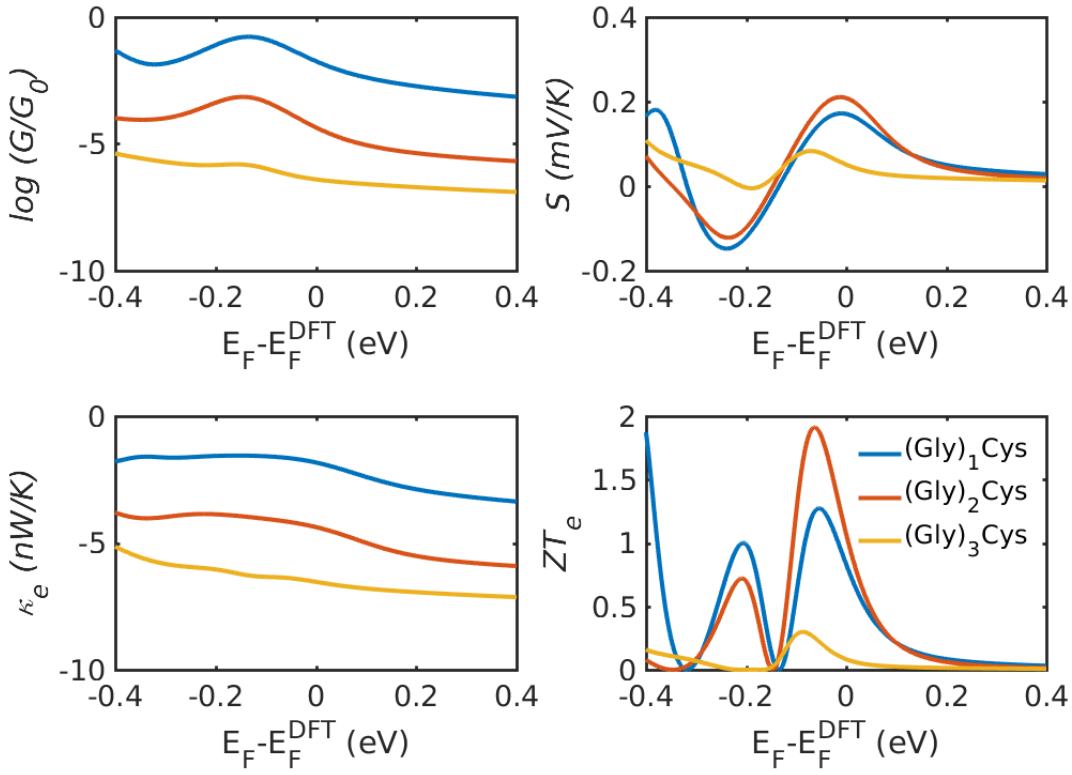


Figure S5. Thermoelectric properties as the function of energy relative to DFT-estimated Fermi energy $E_F - E_F^{DFT}$ at room temperature 300 K for $(Gly)_nCys$ series. (a) Electrical conductance (G), (b) Seebeck coefficients (S), (c)-(d) Electronic contribution to thermal conductance (κ_e) and figure of merit ZT_e . The blue, red and orange curves represent the $(Gly)_1Cys$, $(Gly)_2Cys$ and $(Gly)_3Cys$ junctions respectively.

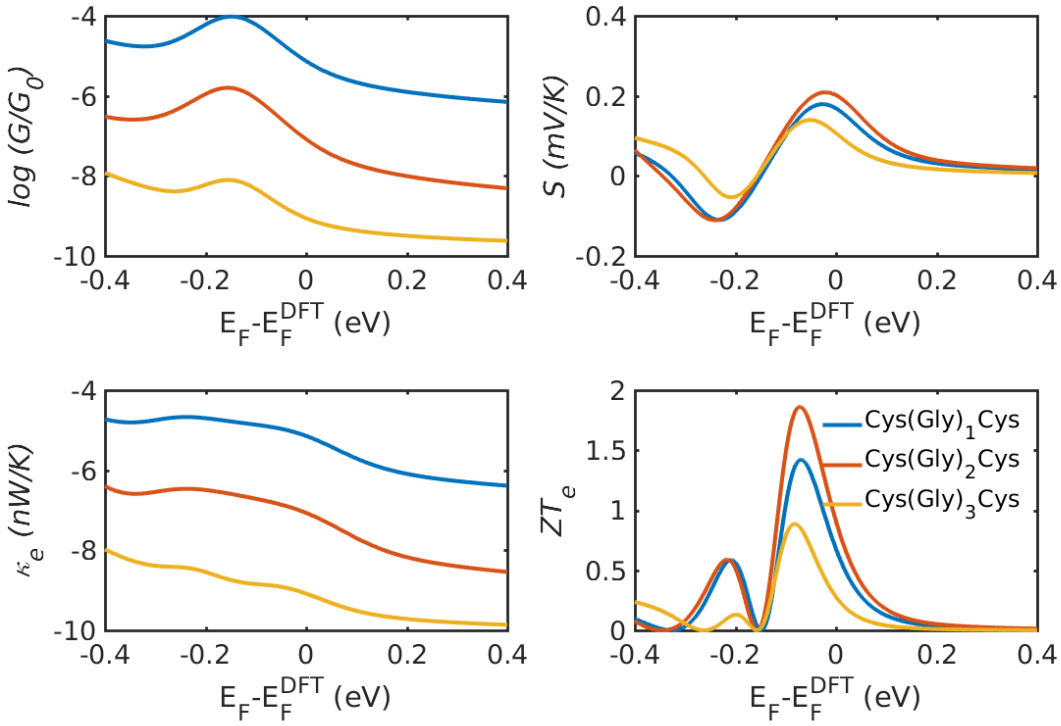


Figure S6. Thermoelectric properties as the function of energy relative to DFT-estimated Fermi energy $E_F - E_F^{DFT}$ at room temperature 300 K for Cys(Gly)$_n$Cys series. (a) Electrical conductance (G), (b) Seebeck coefficients (S), (c)-(d) Electronic contribution to thermal conductance (κ_e) and figure of merit ZT_e . The blue, red and orange curves represent the Cys(Gly)$_1$Cys, Cys(Gly)$_2$Cys and Cys(Gly)$_3$Cys junctions respectively.