

## Electronic Supplementary Information

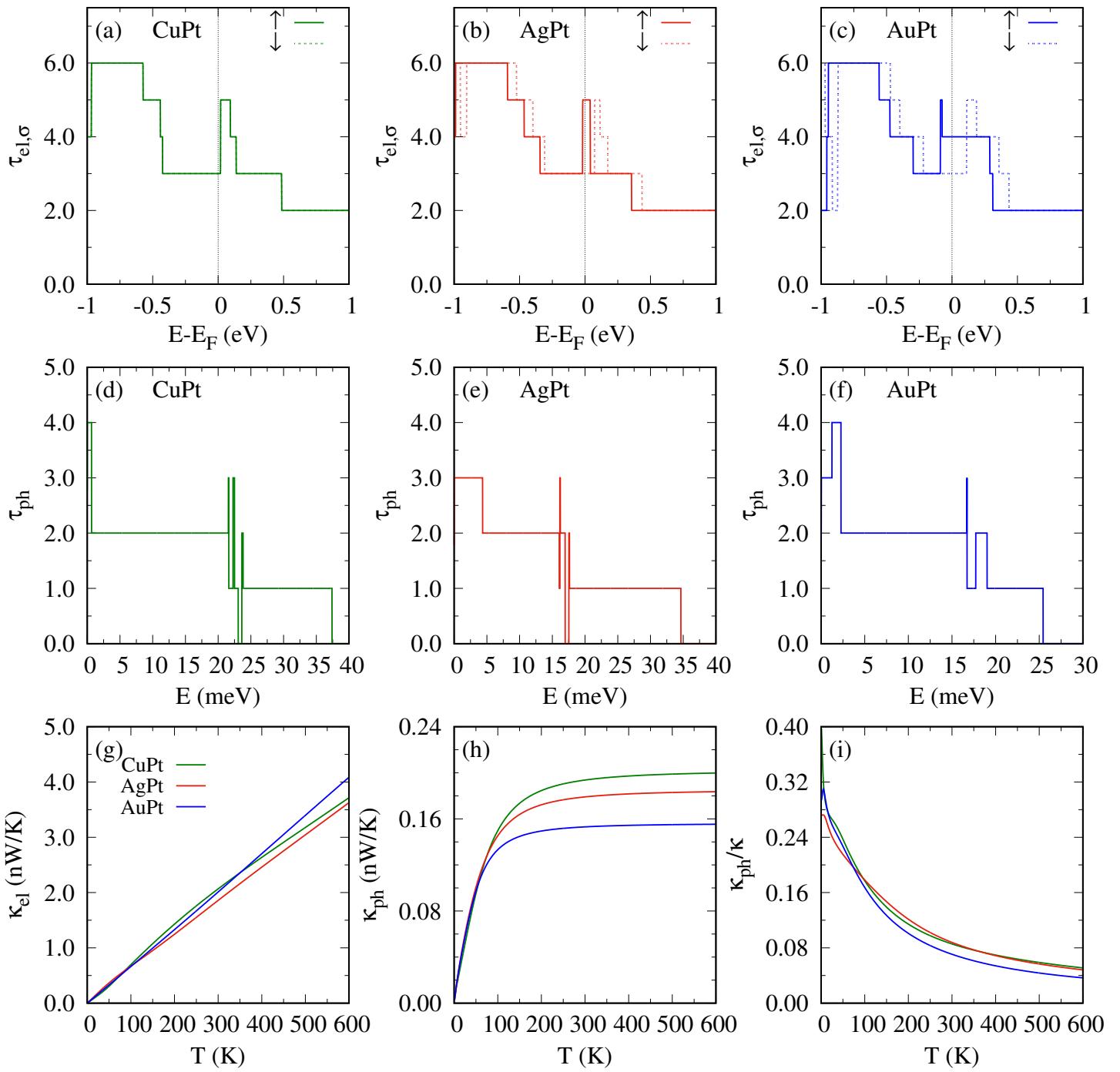
# Alloying-induced Spin Seebeck Effect and Spin Figure of Merit in Pt-based Bimetallic Atomic Wires of Noble Metals

Gurvinder Singh<sup>a,b</sup>, Krishan Kumar<sup>a</sup>, and R. K. Moudgil<sup>b</sup>

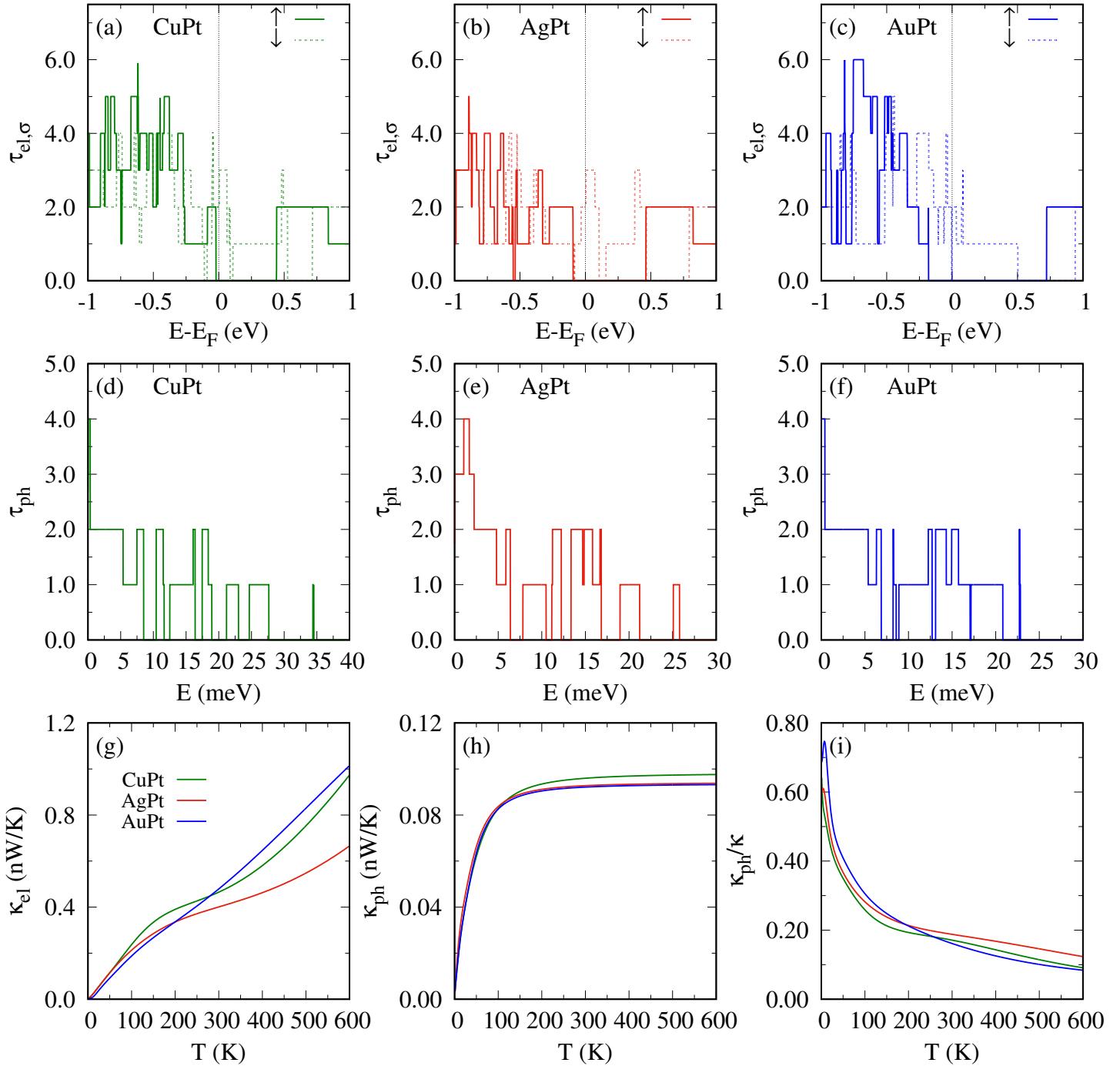
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<sup>b</sup>*Department of Physics, Kurukshetra University, Kurukshetra - 136 119, India.*

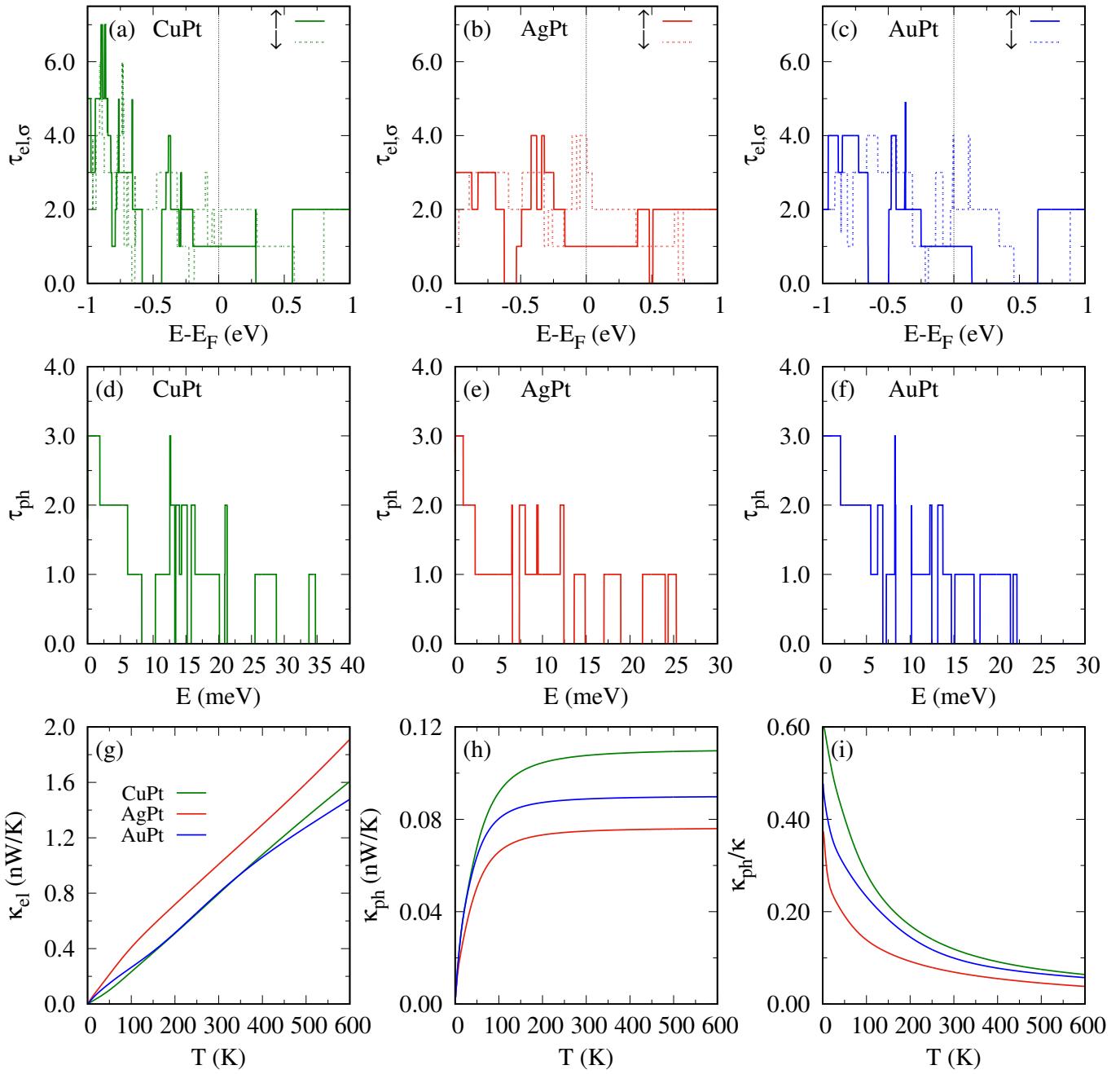
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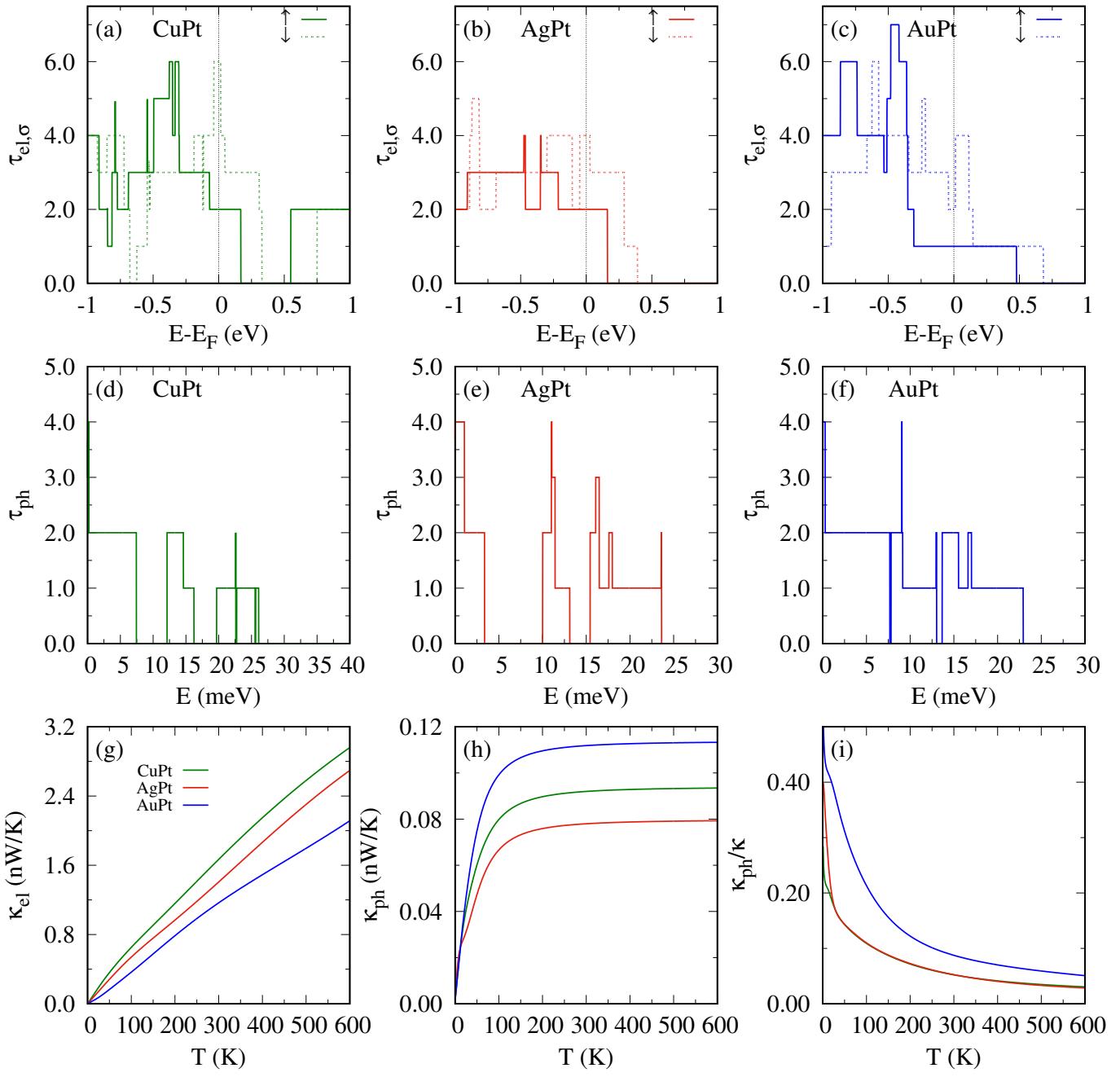
**Figure S1** (Color online) Different transport properties of CuPt, AgPt, and AuPt atomic wires in ladder topology: (a-c) spin-resolved electronic transmission coefficient  $\tau_{el,\sigma}$  plotted as a function of  $(E - E_F)$ ; (d-f) phononic transmission coefficient  $\tau_{ph}$  plotted as a function of phonon energy  $E$ ; (g-i) electronic  $\kappa_{el}$ , phononic  $\kappa_{ph}$ , and relative phononic  $\kappa_{ph}/\kappa$  thermal conductance, respectively, plotted as a function of temperature  $T$  for  $\mu = 0$ .



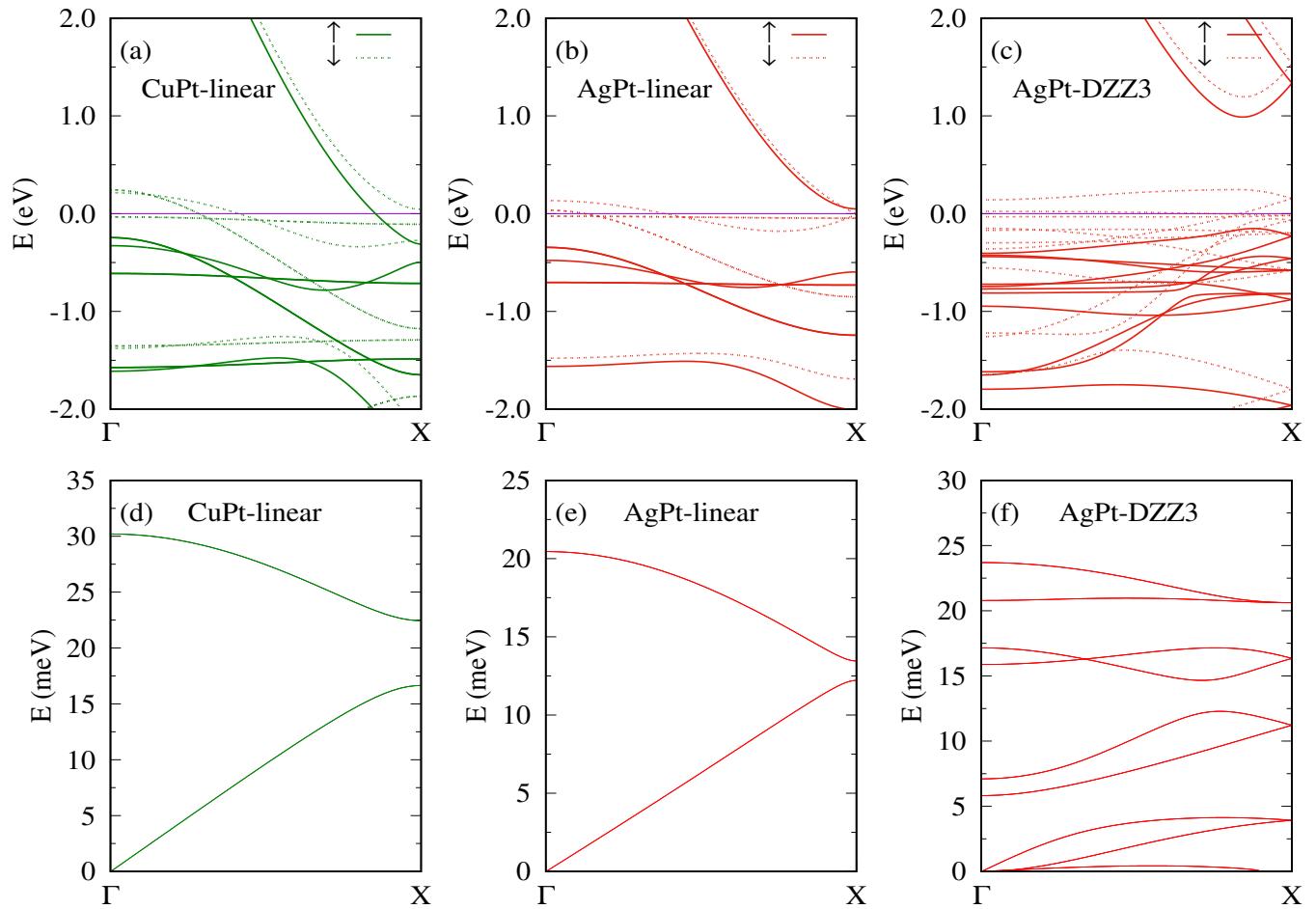
**Figure S2** (Color online) Different transport properties of CuPt, AgPt, and AuPt atomic wires in DZZ1 topology. The curves are labelled in the same manner as in Fig. S1.



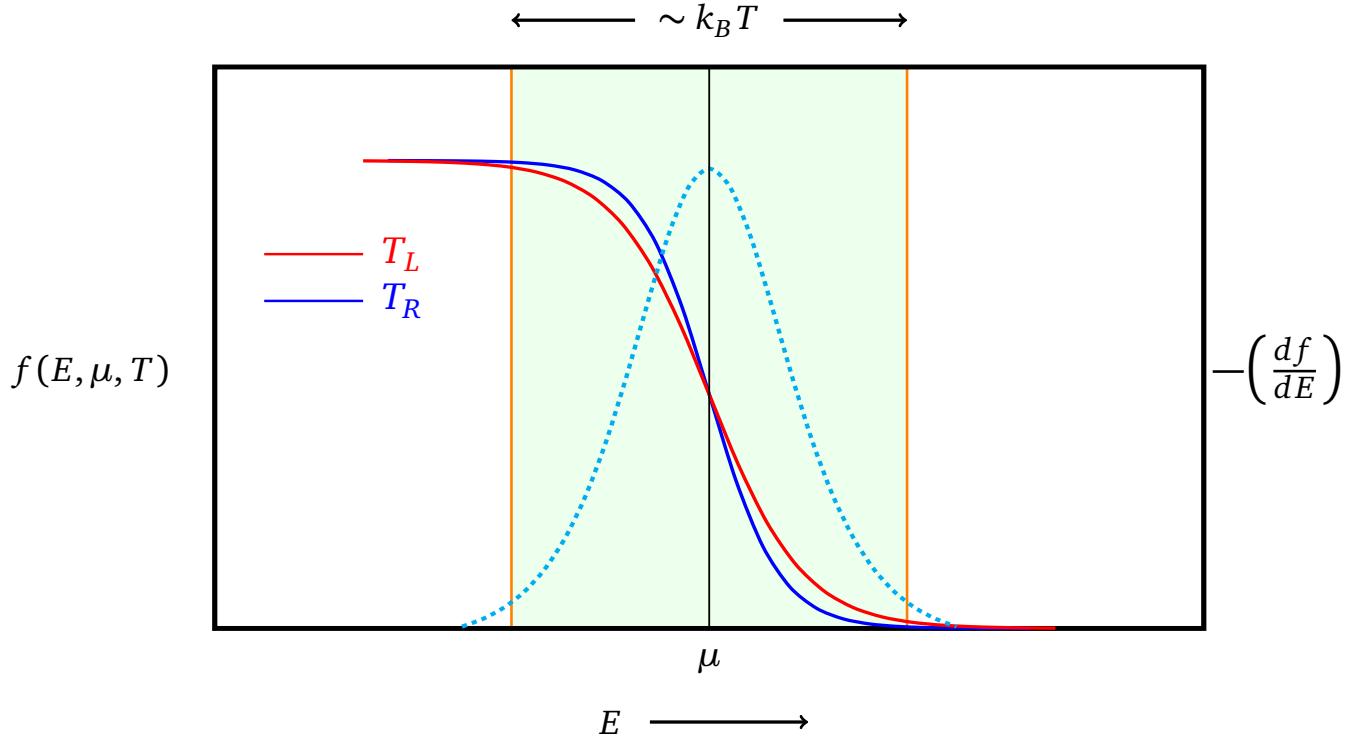
**Figure S3** (Color online) Different transport properties of CuPt, AgPt, and AuPt atomic wires in DZZ2 topology. The curves are labelled in the same manner as in Fig. S1.



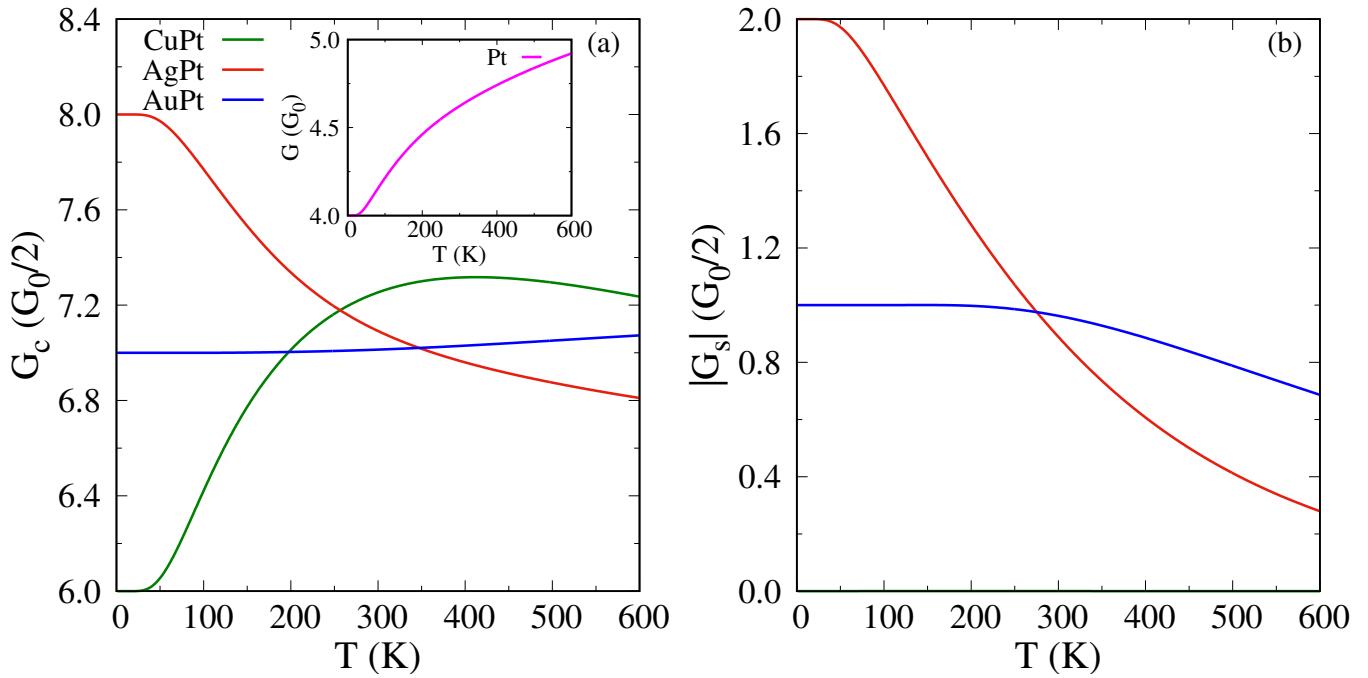
**Figure S4** (Color online) Different transport properties of CuPt, AgPt, and AuPt atomic wires in DZZ4 topology. The curves are labelled in the same manner as in Fig. S1.



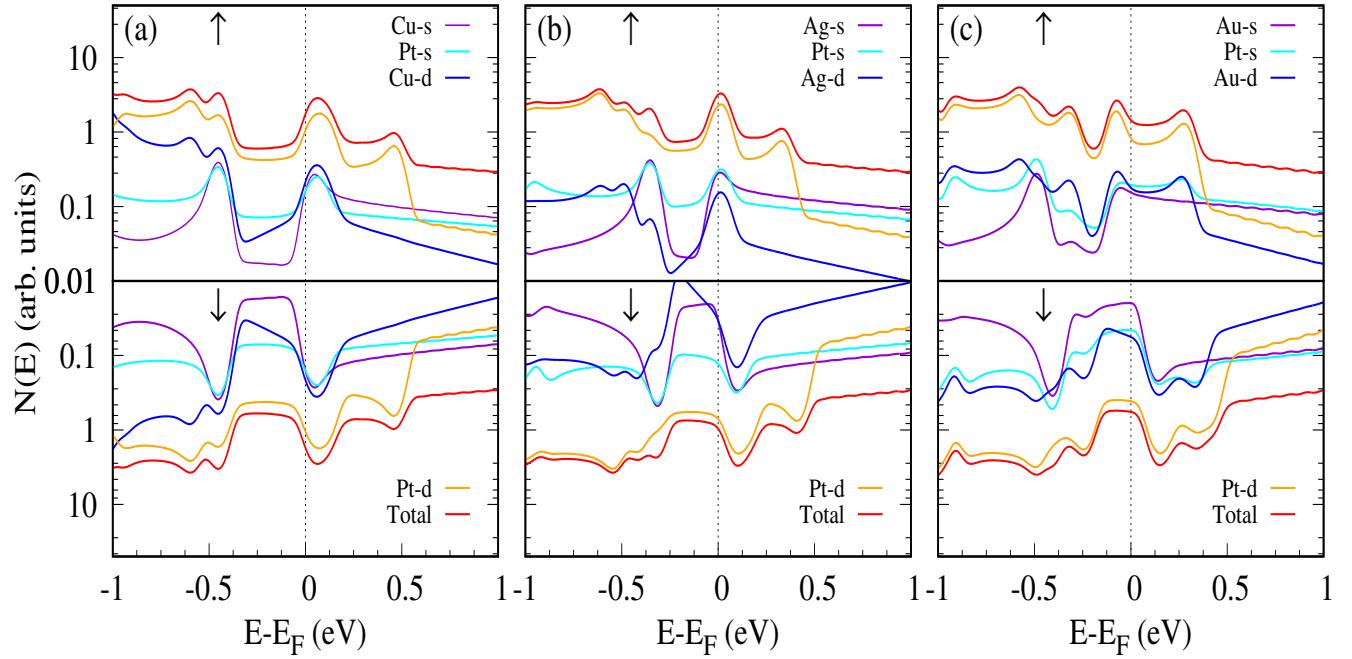
**Figure S5** (Color online) Electronic band structure plots of (a) CuPt-linear, (b) AgPt-linear, and (c) AgPt-DZZ3 atomic wires; the zero of energy is taken at Fermi energy. The panels (d-f) contain the corresponding phononic band structures.



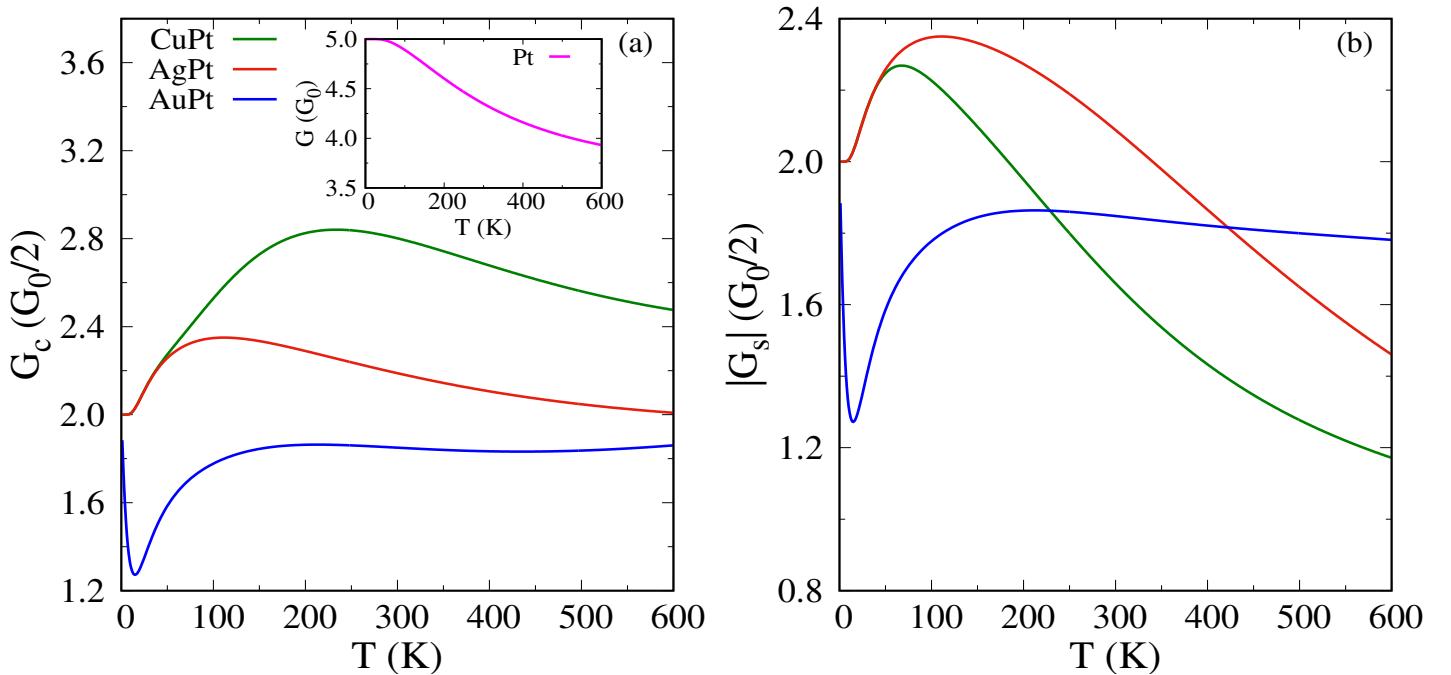
**Figure S6** (Color online) Schematic illustration of the Fermi function  $f(E, \mu, T)$  at two different temperatures  $T_L$  and  $T_R$  ( $T_L > T_R$ ), and  $-df/dE$  at a given temperature  $T$  (dashed line).



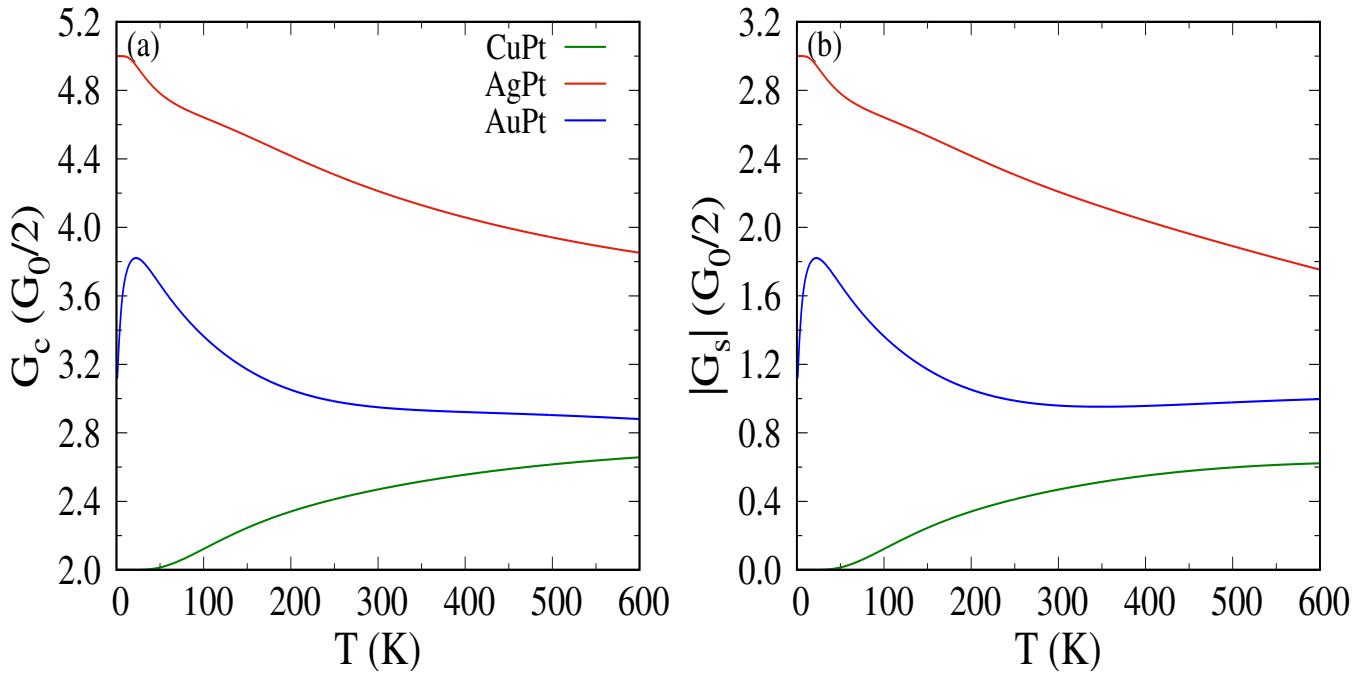
**Figure S7** (Color online) (a) Charge  $G_c$  and (b) spin  $|G_s|$  electrical conductance plotted as a function of temperature  $T$  for different bimetallic atomic wires in ladder topology. The inset in (a) depicts electrical conductance  $G$  for the pristine Pt wire in ladder topology.



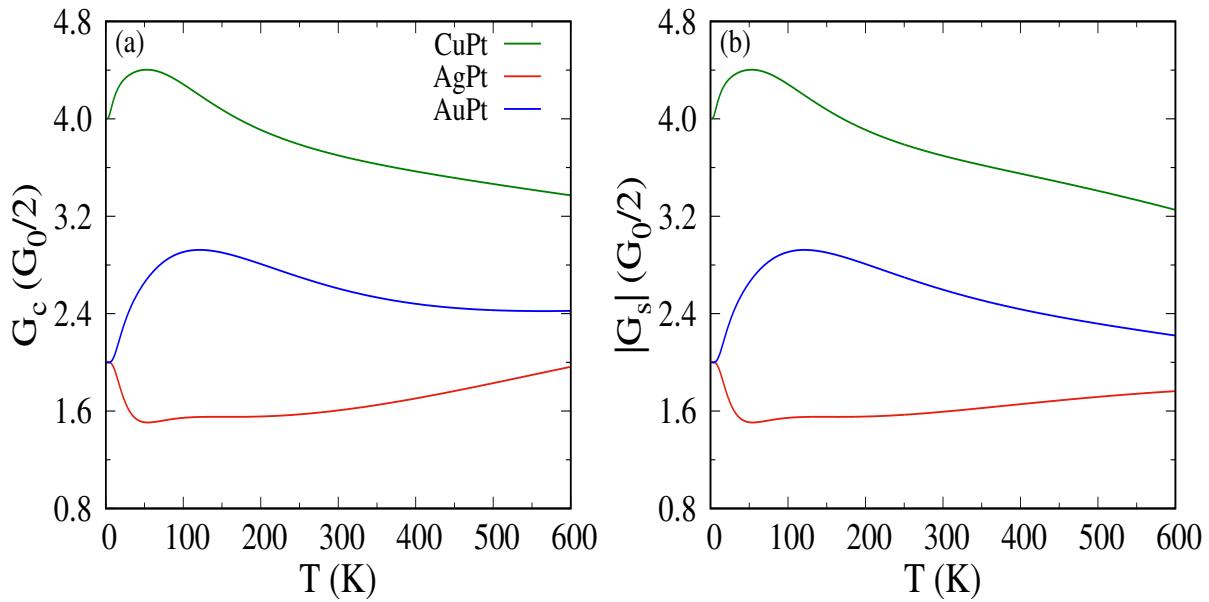
**Figure S8** (Color online) The orbital-resolved and total density of  $\uparrow$ - (in upper half) and  $\downarrow$ -spin (in lower half) states for (a) CuPt, (b) AgPt, and (c) AuPt atomic wires in ladder topology.



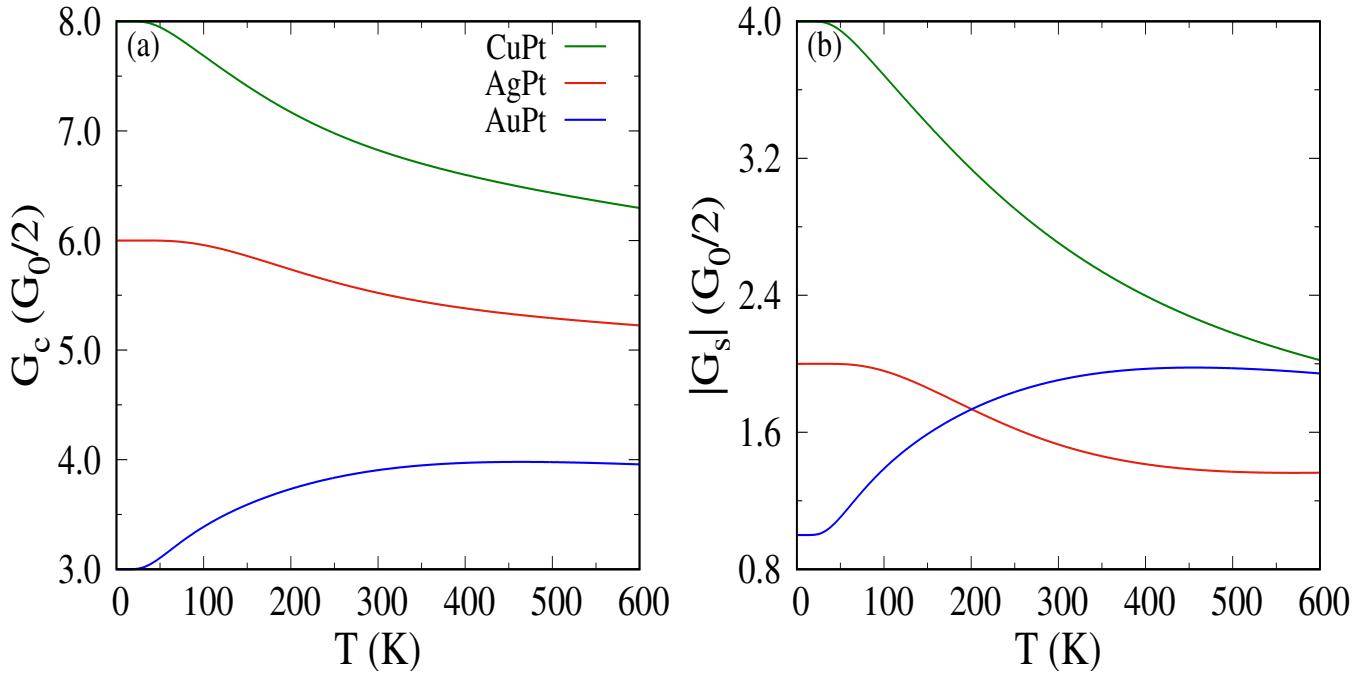
**Figure S9** (Color online) (a) Charge  $G_c$  and (b) spin  $|G_s|$  electrical conductance plotted as a function of temperature  $T$  for different bimetallic atomic wires in DZZ1 topology. The inset in (a) depicts electrical conductance  $G$  for the pristine Pt wire in DZZ topology.



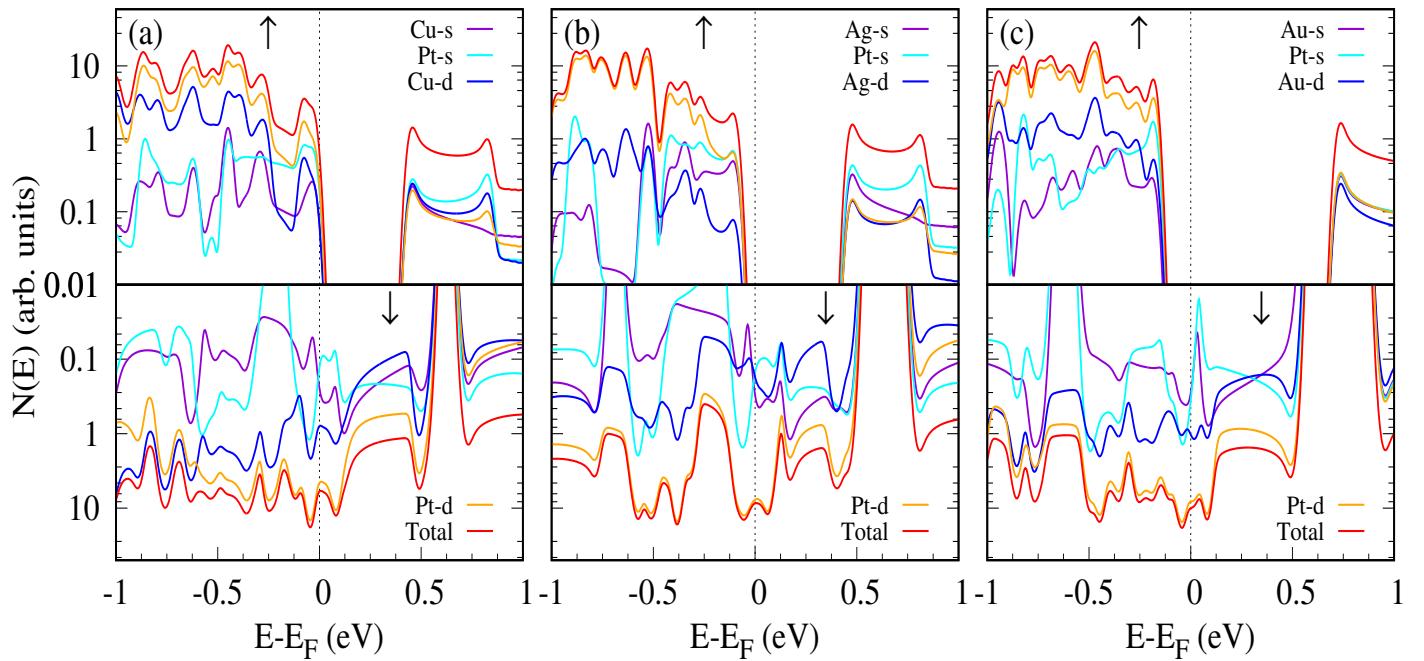
**Figure S10** (Color online) (a) Charge  $G_c$  and (b) spin  $|G_s|$  electrical conductance plotted as a function of temperature  $T$  for different bimetallic wires in DZZ2 topology.



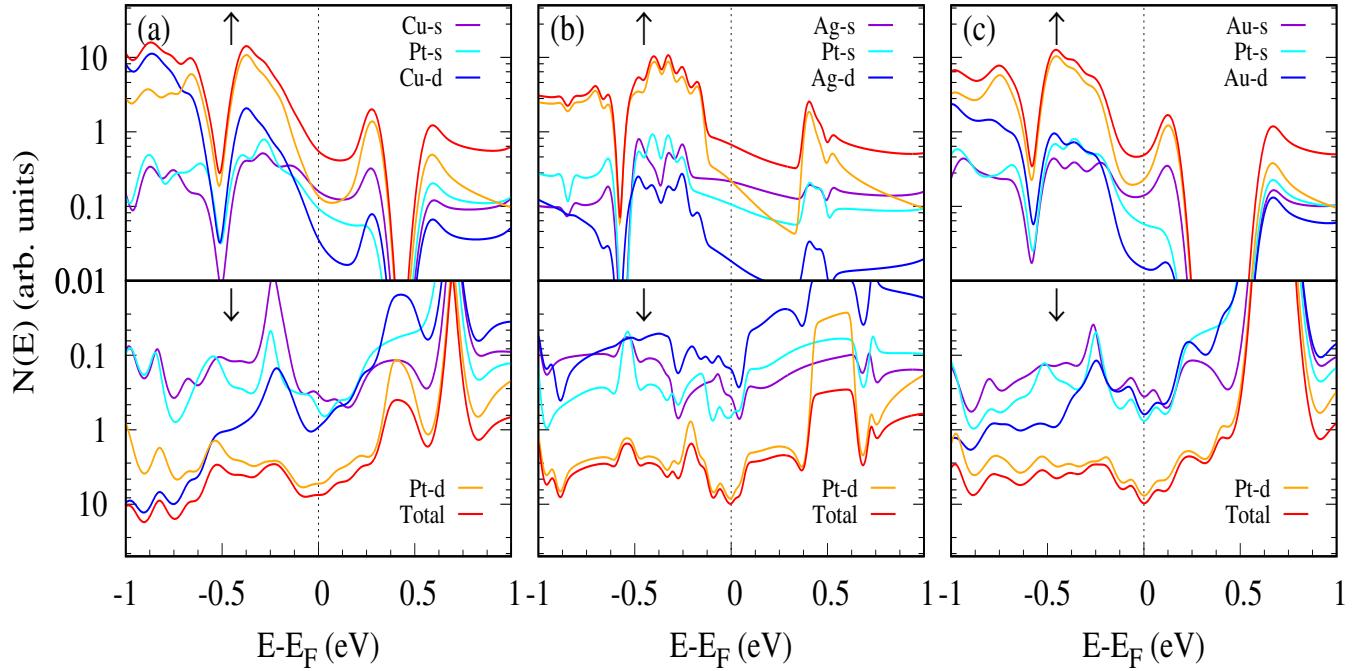
**Figure S11** (Color online) (a) Charge  $G_c$  and (b) spin  $|G_s|$  electrical conductance plotted as a function of temperature  $T$  for different bimetallic wires in DZZ3 topology.



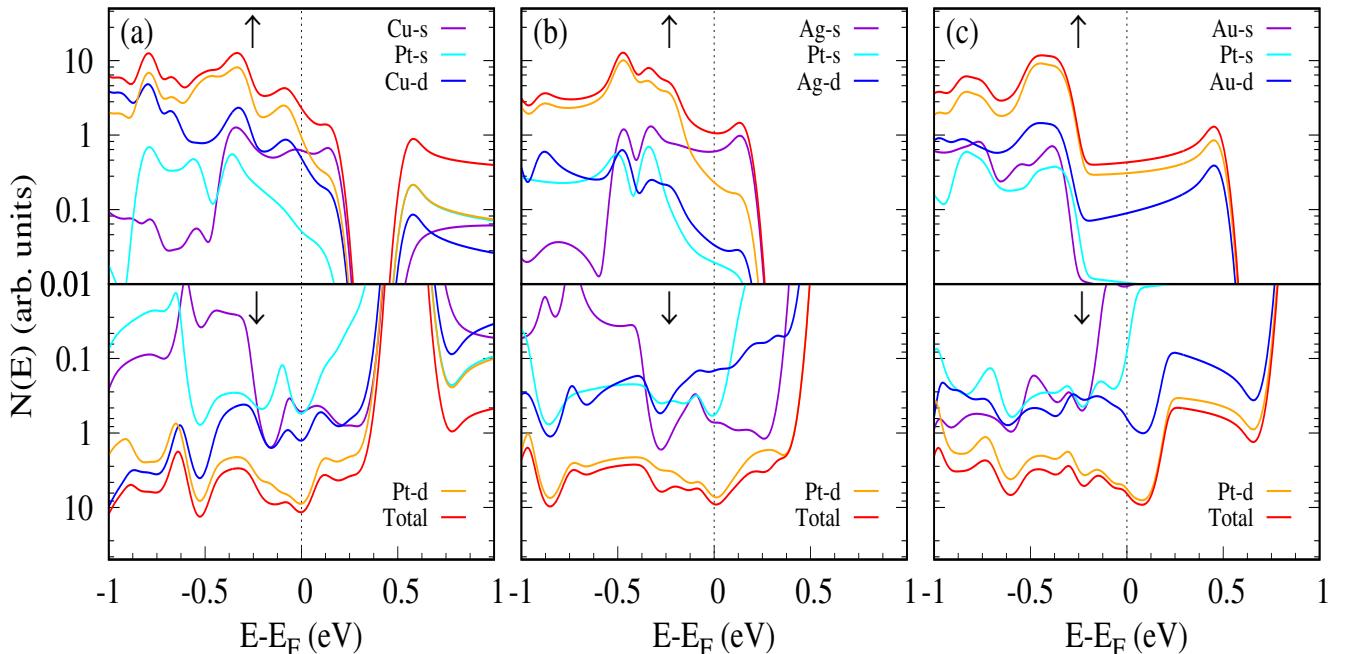
**Figure S12** (Color online) (a) Charge  $G_c$  and (b) spin  $|G_s|$  electrical conductance plotted as a function of temperature  $T$  for different bimetallic wires in DZZ4 topology.



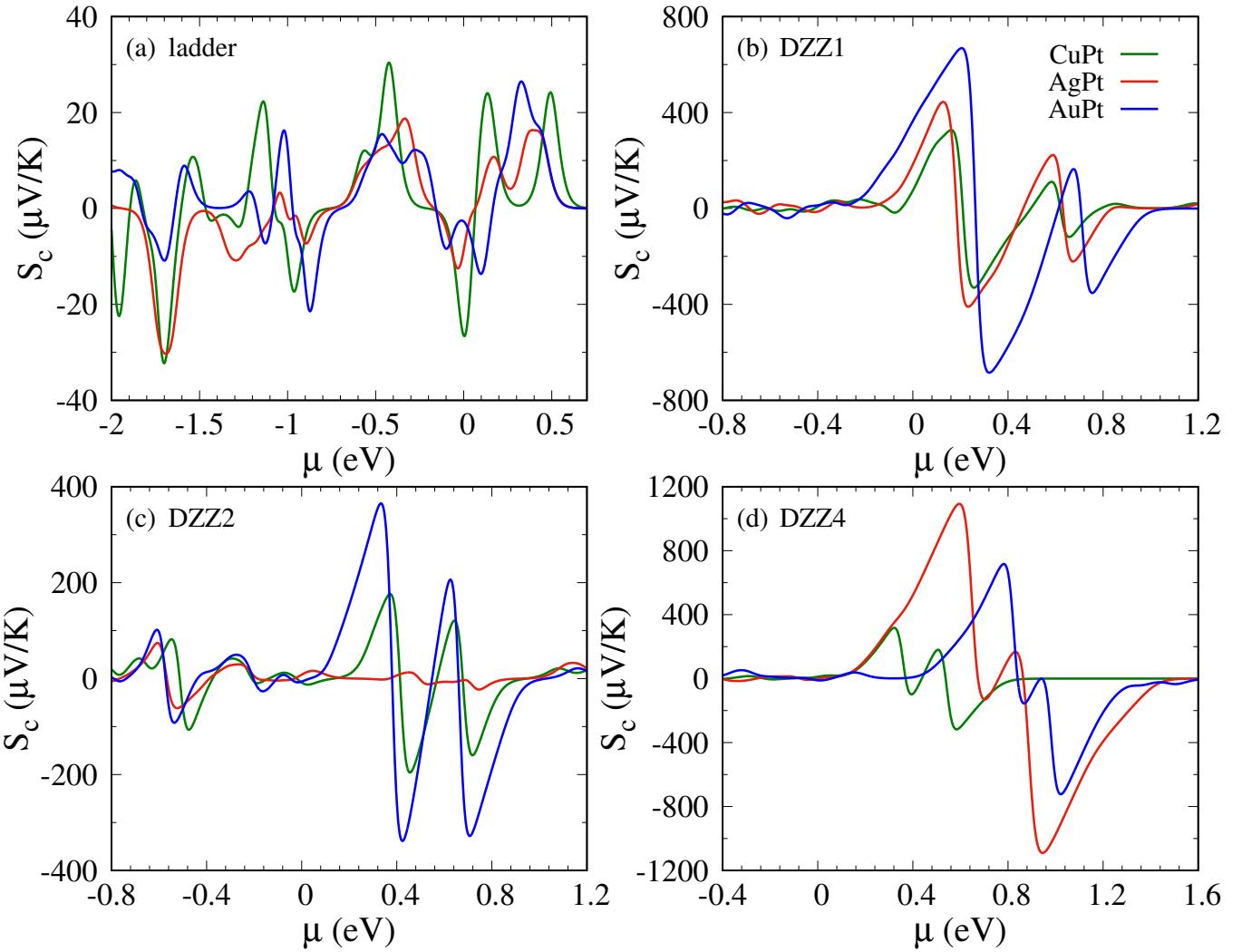
**Figure S13** (Color online) The orbital-resolved and total density of  $\uparrow$ - (in upper half) and  $\downarrow$ -spin (in lower half) states for (a) CuPt, (b) AgPt, and (c) AuPt atomic wires in DZZ1 topology.



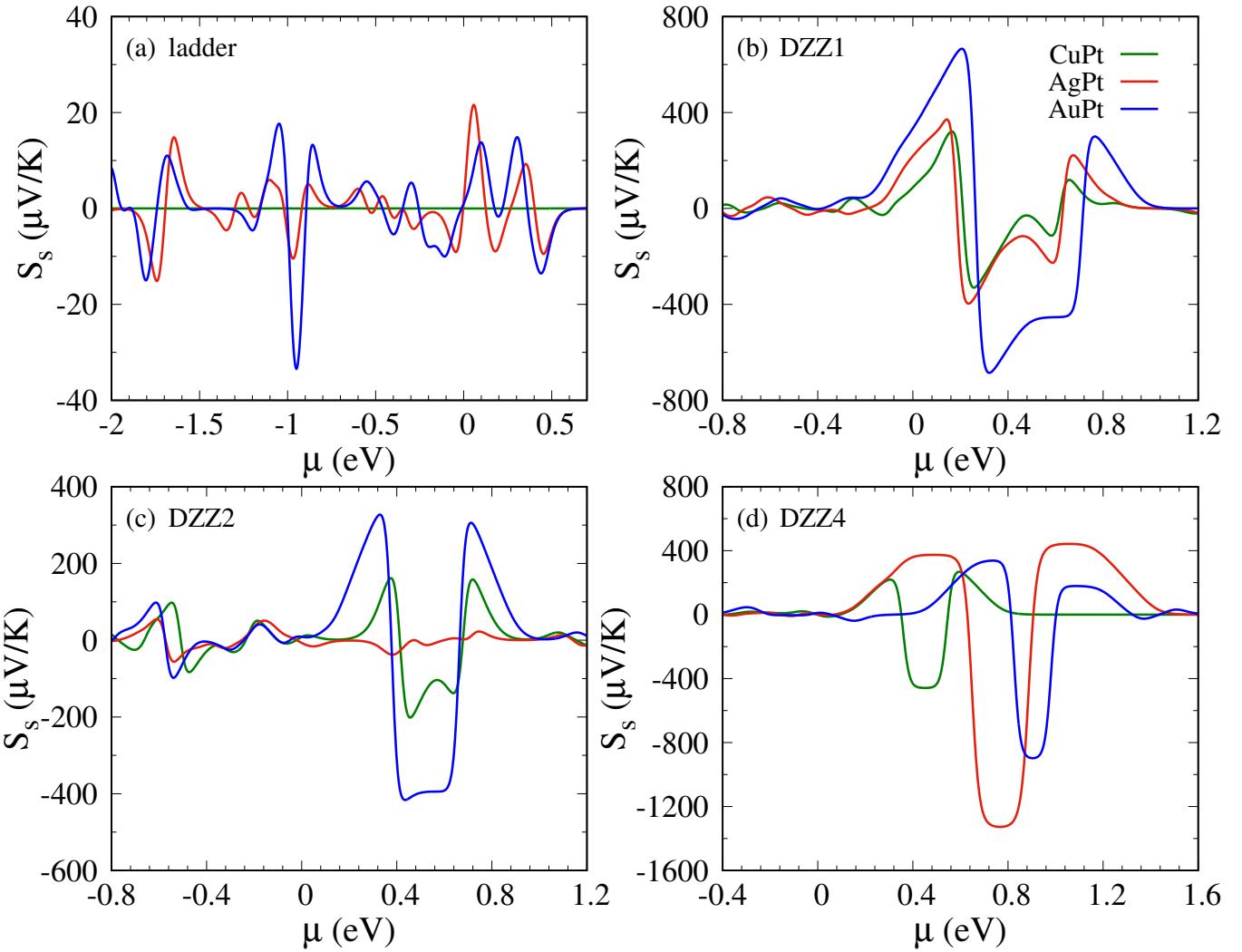
**Figure S14** (Color online) The orbital-resolved and total density of  $\uparrow$ - (in upper half) and  $\downarrow$ -spin (in lower half) states for (a) CuPt, (b) AgPt, and (c) AuPt atomic wires in DZZ2 topology.



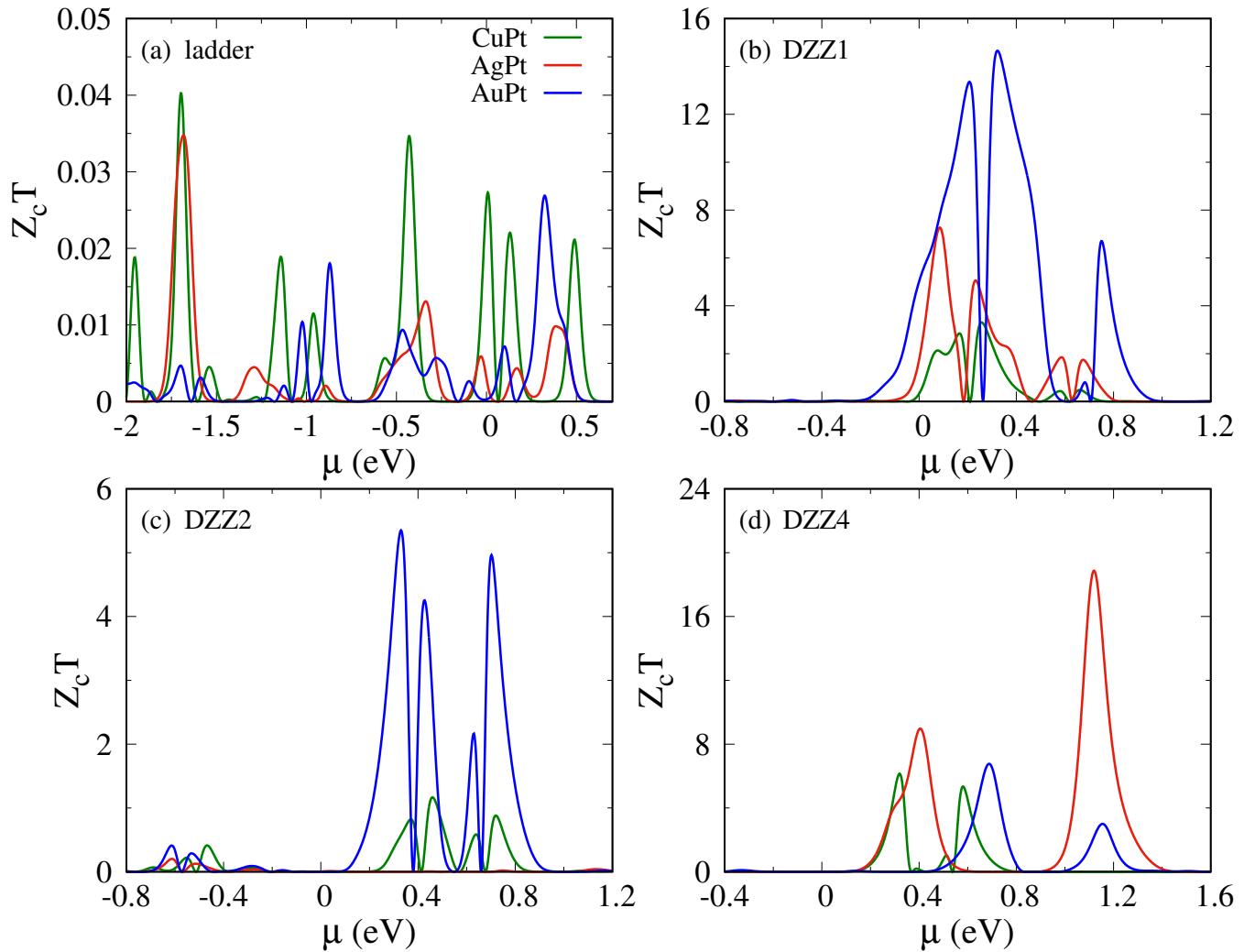
**Figure S15** (Color online) The orbital-resolved and total density of  $\uparrow$ - (in upper half) and  $\downarrow$ -spin (in lower half) states for (a) CuPt, (b) AgPt, and (c) AuPt atomic wires in DZZ4 topology.



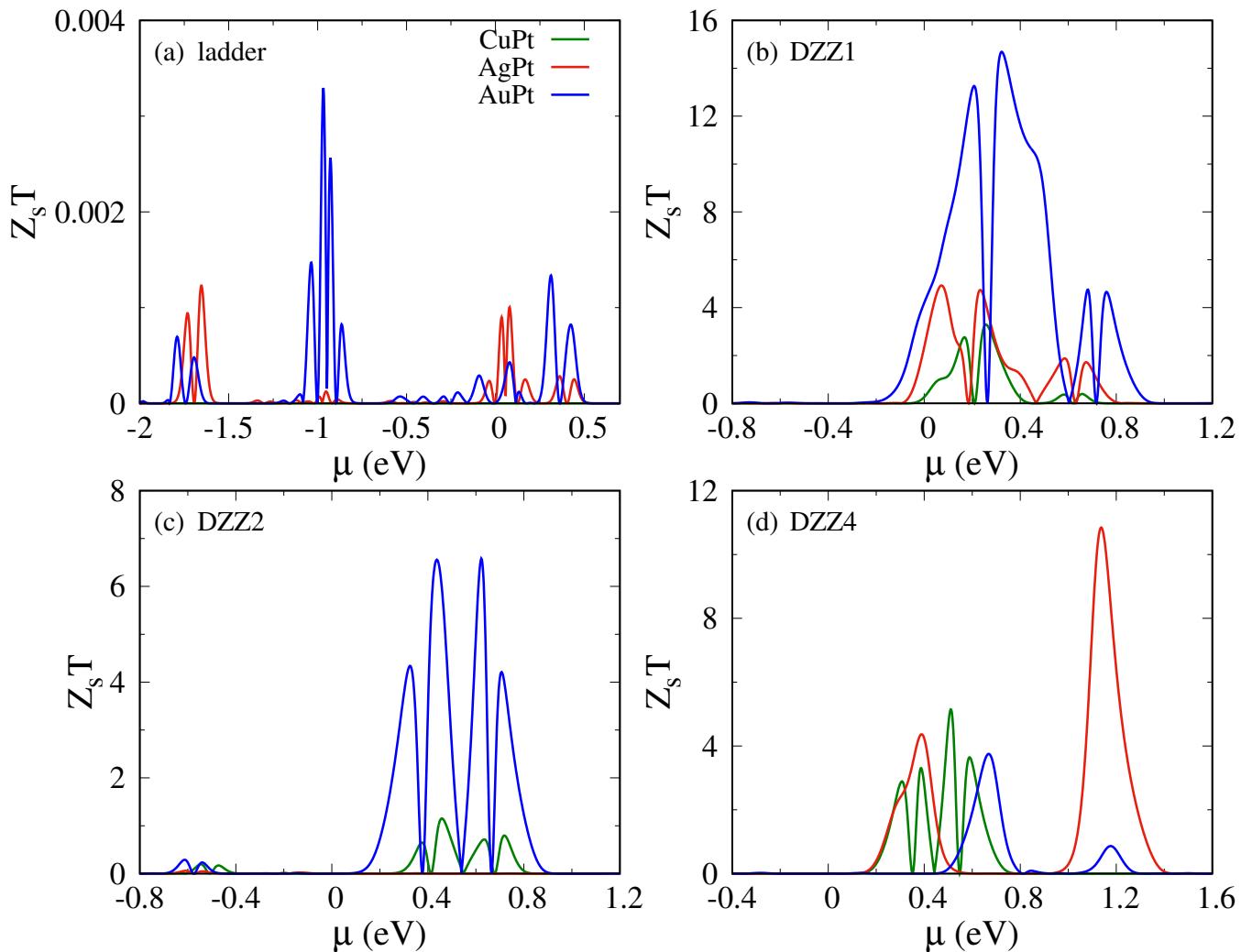
**Figure S16** (Color online) Charge Seebeck coefficient  $S_c$  plotted as a function of chemical potential  $\mu$  for different bimetallic wires in (a) ladder, (b) DZZ1, (c) DZZ2, and (d) DZZ4 topologies.



**Figure S17** (Color online) Spin Seebeck coefficient  $S_s$  plotted as a function of chemical potential  $\mu$  for different bimetallic wires in (a) ladder, (b) DZZ1, (c) DZZ2, and (d) DZZ4 topologies.



**Figure S18** (Color online) Charge figure of merit  $Z_c T$  plotted as a function of chemical potential  $\mu$  for different bimetallic wires in (a) ladder, (b) DZZ1, (c) DZZ2, and (d) DZZ4 topologies.



**Figure S19** (Color online) Spin figure of merit  $Z_s T$  plotted as a function of chemical potential  $\mu$  for different bimetallic wires in (a) ladder, (b) DZZ1, (c) DZZ2, and (d) DZZ4 topologies.