Supporting Information

Identification of a positive-Seebeck-coefficient exohedral fullerene

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Table S1. DFT calculation of the charge transferred between the chlorine atoms and fullerene C_{50}.

	Neutral	With Cl	ΔN
C_{50}	200	198.67	+1.32
Cl_{10}	70	71.318	-1.318

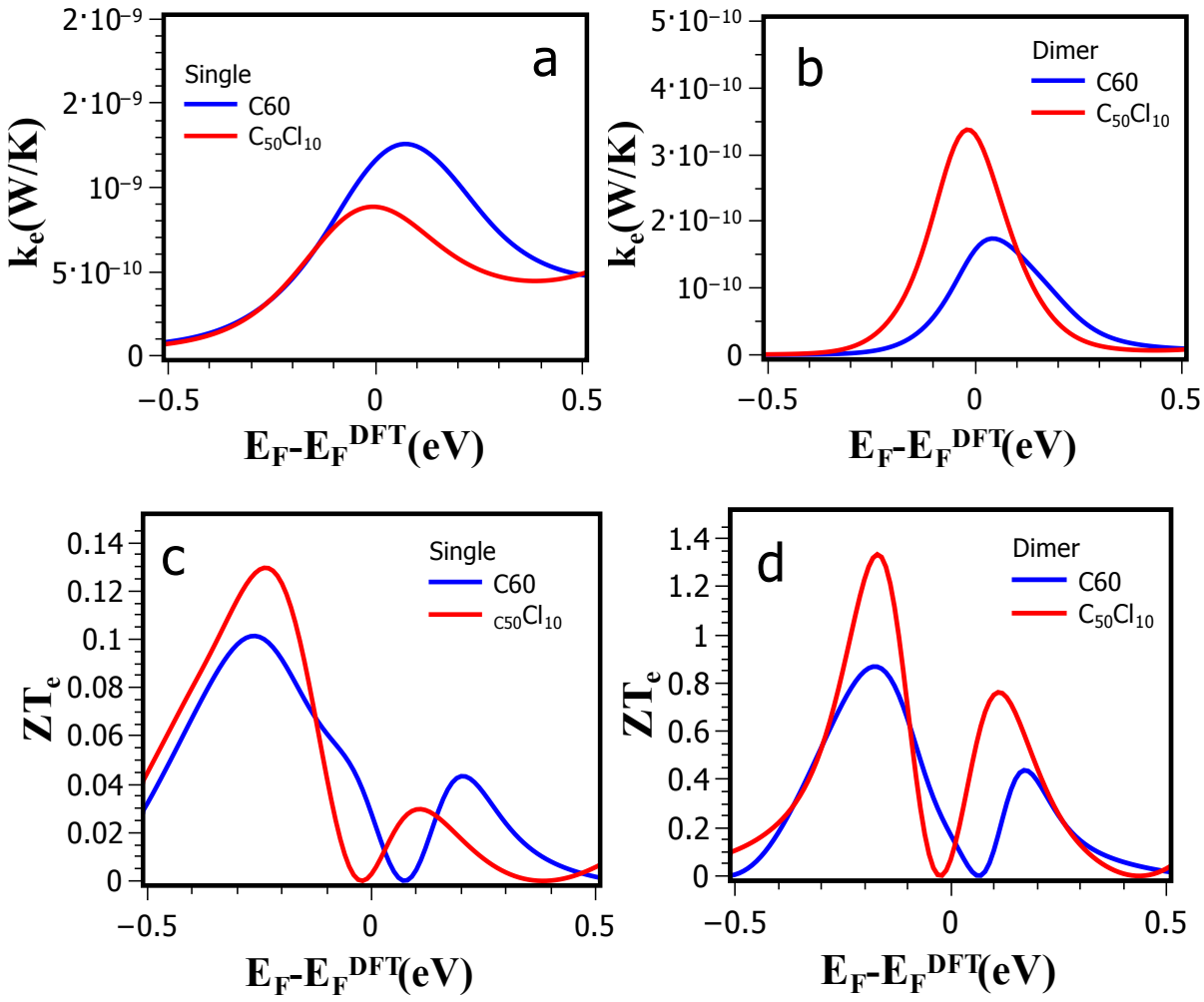

Figure S1. The upper panel, Figures (a and b) shows a comparison of room-temperature electronic thermal conductance (k_e) and the lower panel, Figures (c and d) show electronic figure of merit (ZT_e) over a range of Fermi energies E_F relative to the DFT-predicted Fermi energy E_F^{DFT} between for the systems in Figures 3 and 4.

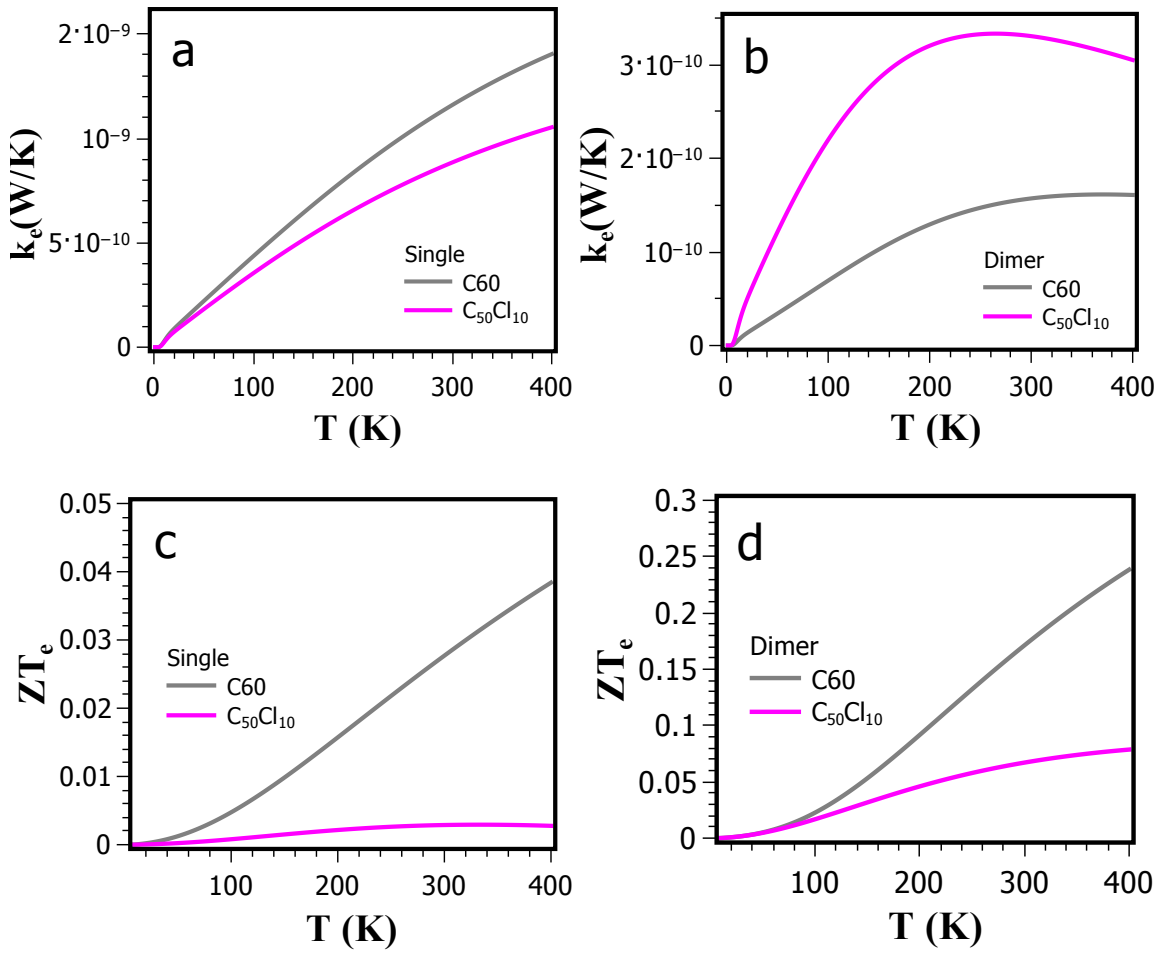

Figure S2. The left column, (a and c) shows a comparison of electronic thermal conductance (k_e) and electronic figure of merit (ZT_e) as a function of temperature at DFT-predicted Fermi energy E_F^{DFT} between the systems in Figures 3a and 4a. The upper panels (a and b) show the comparison of electronic thermal conductance (k_e) the lower panels (c and d) show electronic figure of merit (ZT_e) for the systems in Figures 3b and 4b.

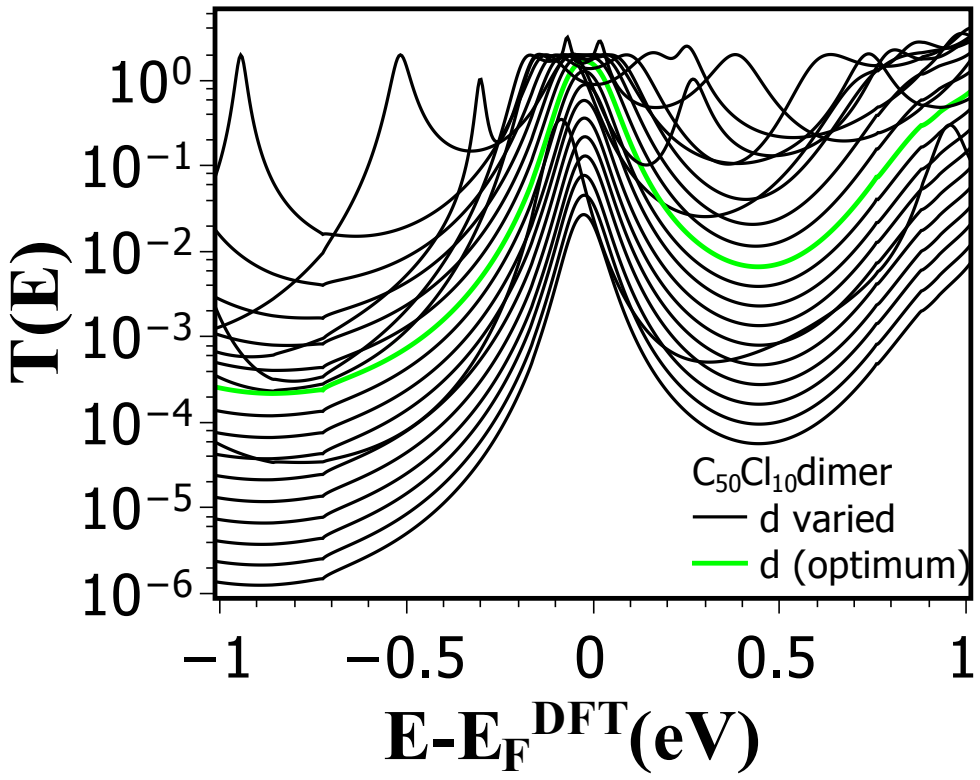

Figure S3. Shows the set of transmission coefficients as a function of energy for $C_{50}Cl_{10}$ dimers, where the black lines show *T(E)* for various distances d, ranging from 1.2 Å to 5 Å. The the green line shows *T(E)* at the optimum distance.