Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for Charge and Spin Thermoelectric Transport in Benzene-Based Molecular Nano-Junctions: A Quantum Many-Body Study

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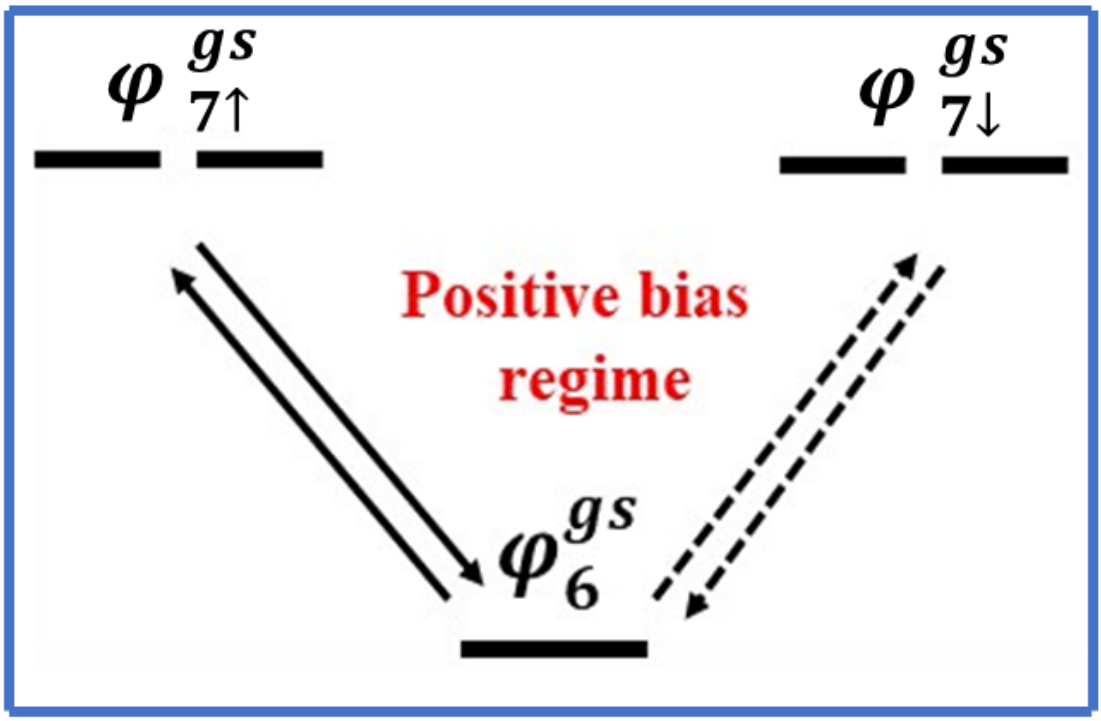

Figure S 1. Sketch of the energetics for the $6 \rightarrow 7$ transition in benzene (positive bias regime). The bold line represents the appropriate possible transitions for which current flow occurs, while the dotted line (only for ortho and meta-connections) represents the forbidden transitions that result in a current blocking situation yielding NDC at specific bias ranges. There is no current-blocking state in the para connection of benzene.

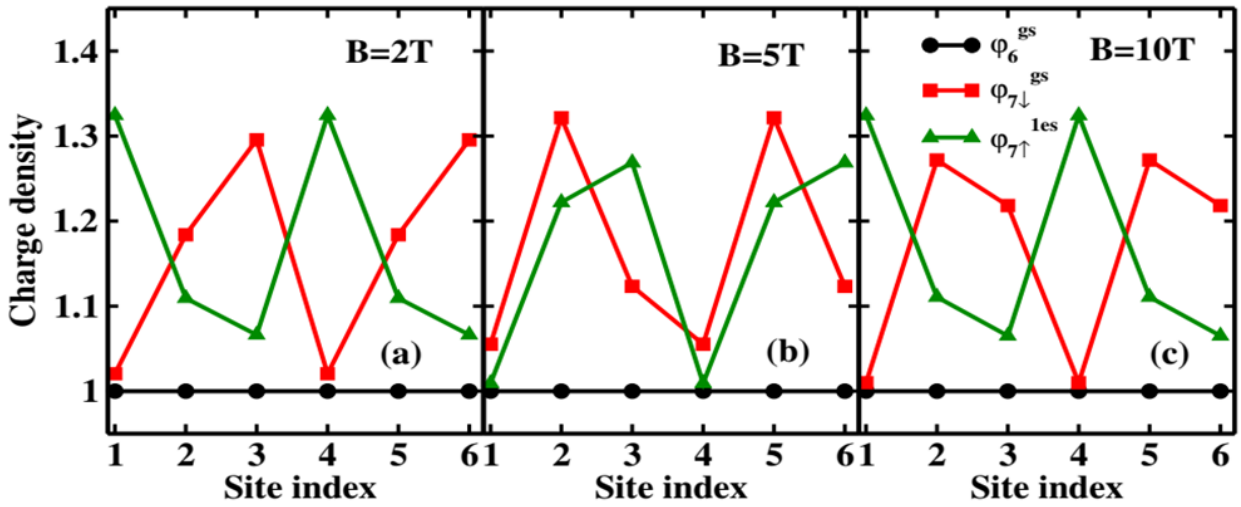

Figure S 2. The charge density distribution of 6-electron ground state (ϕ_6^{gs}), spin down and spin up of 7-electron ground state ($\phi_{7\downarrow}^{gs}$) and first excited state ($\phi_{7\uparrow}^{1es}$) over the sites of benzene at (a) $B = 2T$,(b) $B = 5T$ and (c) $B = 10T$ respectively.

Table S I. 6e-gs and 7e-gs energy level splitting in benzene molecule weakly coupled to normal electrode at different magnetic field (B). Note: in NE, $\phi_{7\uparrow}^{1es}$ will be $\phi_{7\uparrow}^{gs}$.

Electrode	ϕ_6^{gs}	$\phi_{7\downarrow}^{gs}$	$\phi_{7\uparrow}^{1es}$
NE	-30.73	-25.68	-25.68
NE (B=2T)	-30.73	-25.91	-25.45
NE (B=5T)	-30.73	-26.25	-25.10
NE (B=10T)	-30.73	-26.83	-24.53

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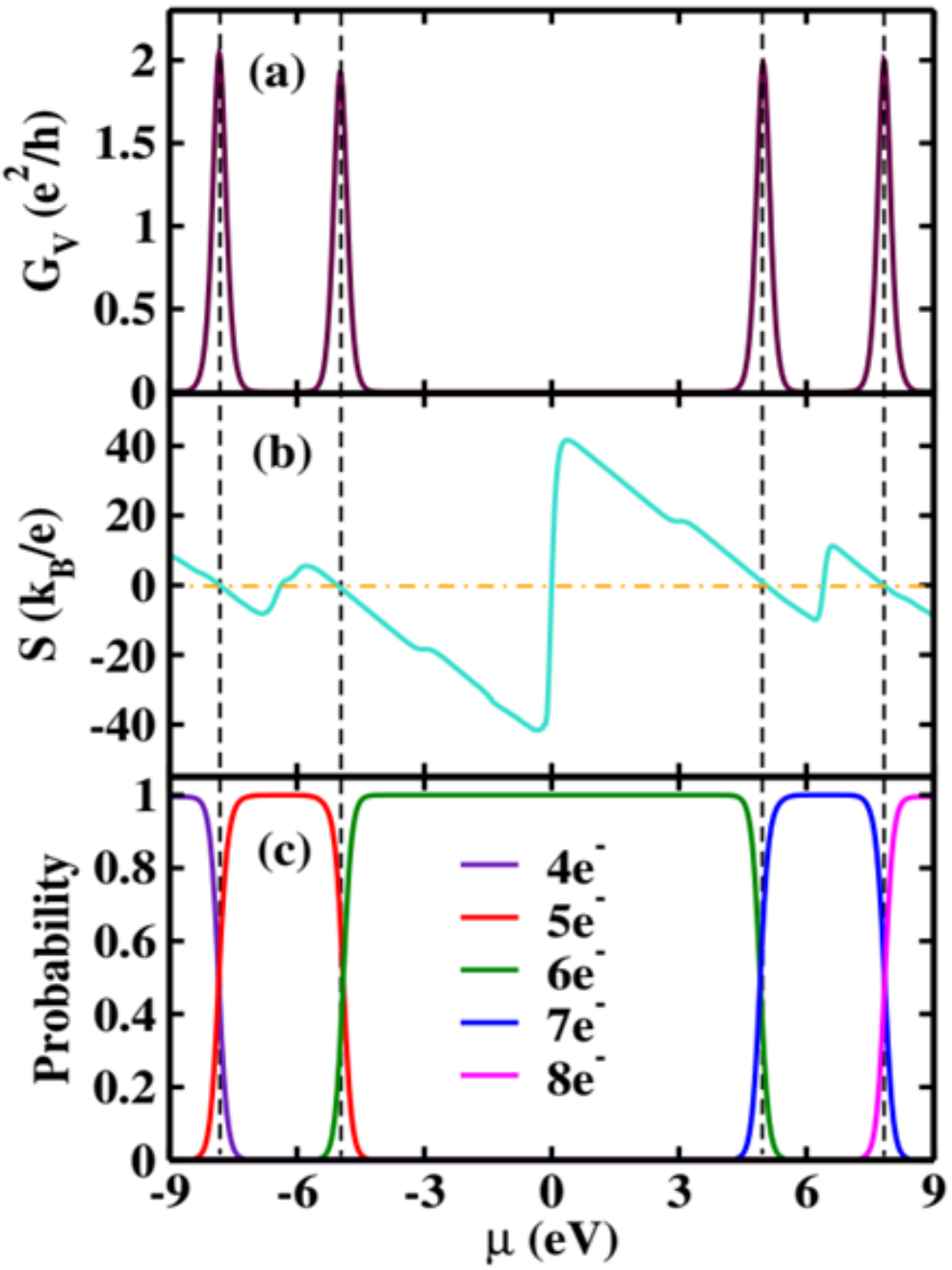

Figure S 3. (a) The electrical conductance, (b) Seebeck coefficient, and (c) the probabilities of occupying $4e^-$, $5e^-$, $6e^-$, $7e^-$ and $8e^-$ states as a function of chemical potential (μ) at $k_BT = 0.1eV$.

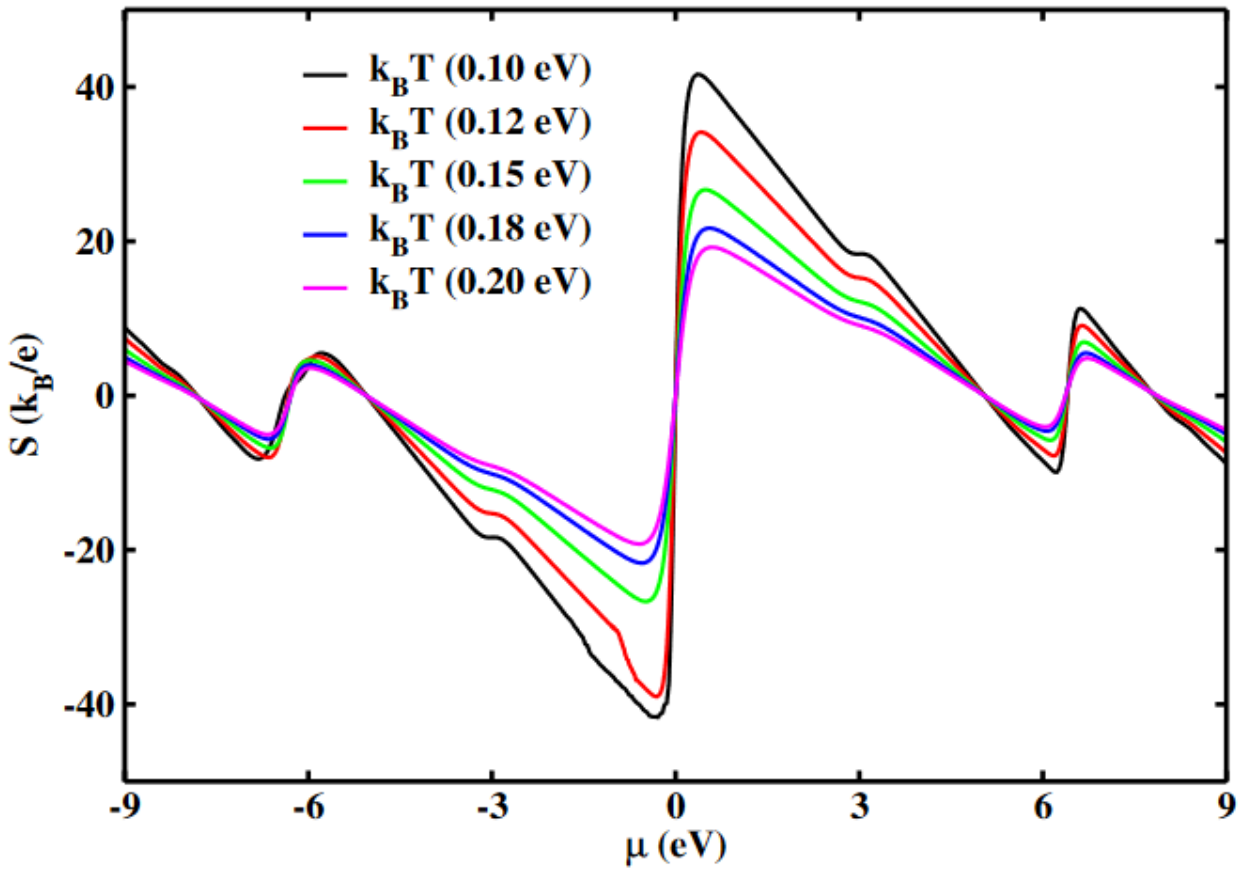

Figure S 4. The 2D plot of charge Seebeck coefficient as a function of different chemical potentials with varying five different temperatures showing saw-tooth pattern.

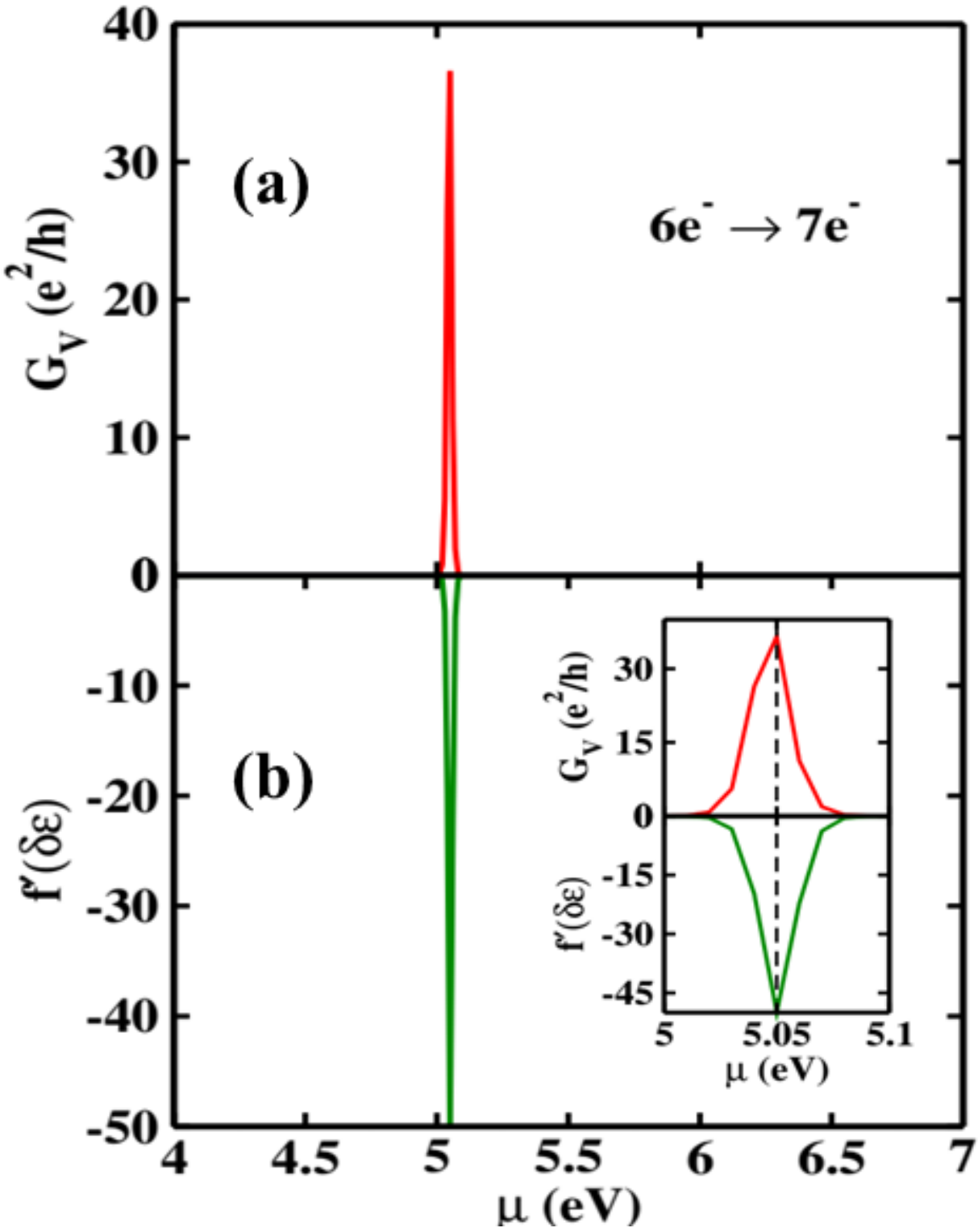

Figure S 5. (a) Represents the 2D plot of electrical conductance (b) derivative of Fermi-Dirac distribution ($f'(\delta\varepsilon)$, where ε is transition energy) as a function of μ at $T = 0.005k_BT$ (only taking the 6→7 transition). The inset of the figure provides a magnified view of a specific region.

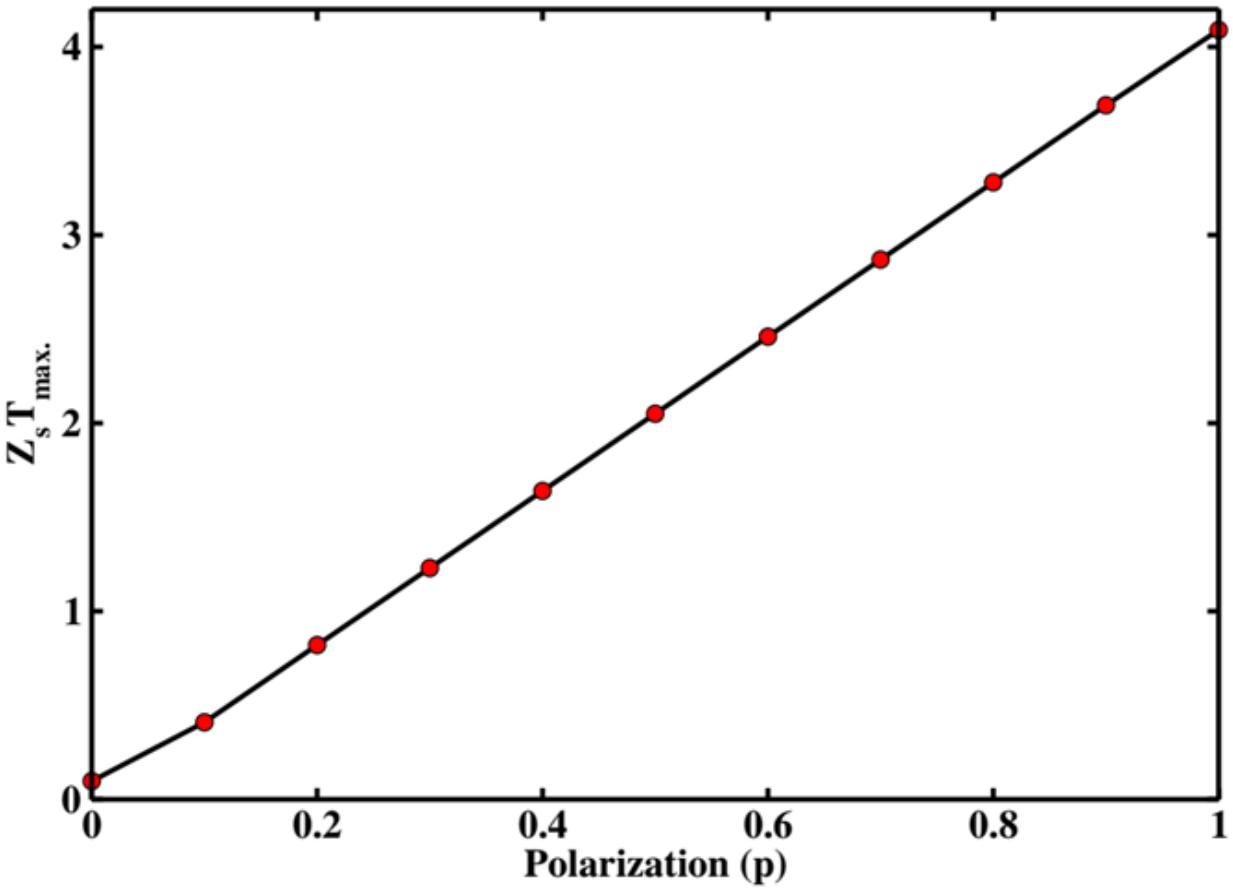

Figure S 6. The maximum value of Z_sT as a function of different polarization (p).

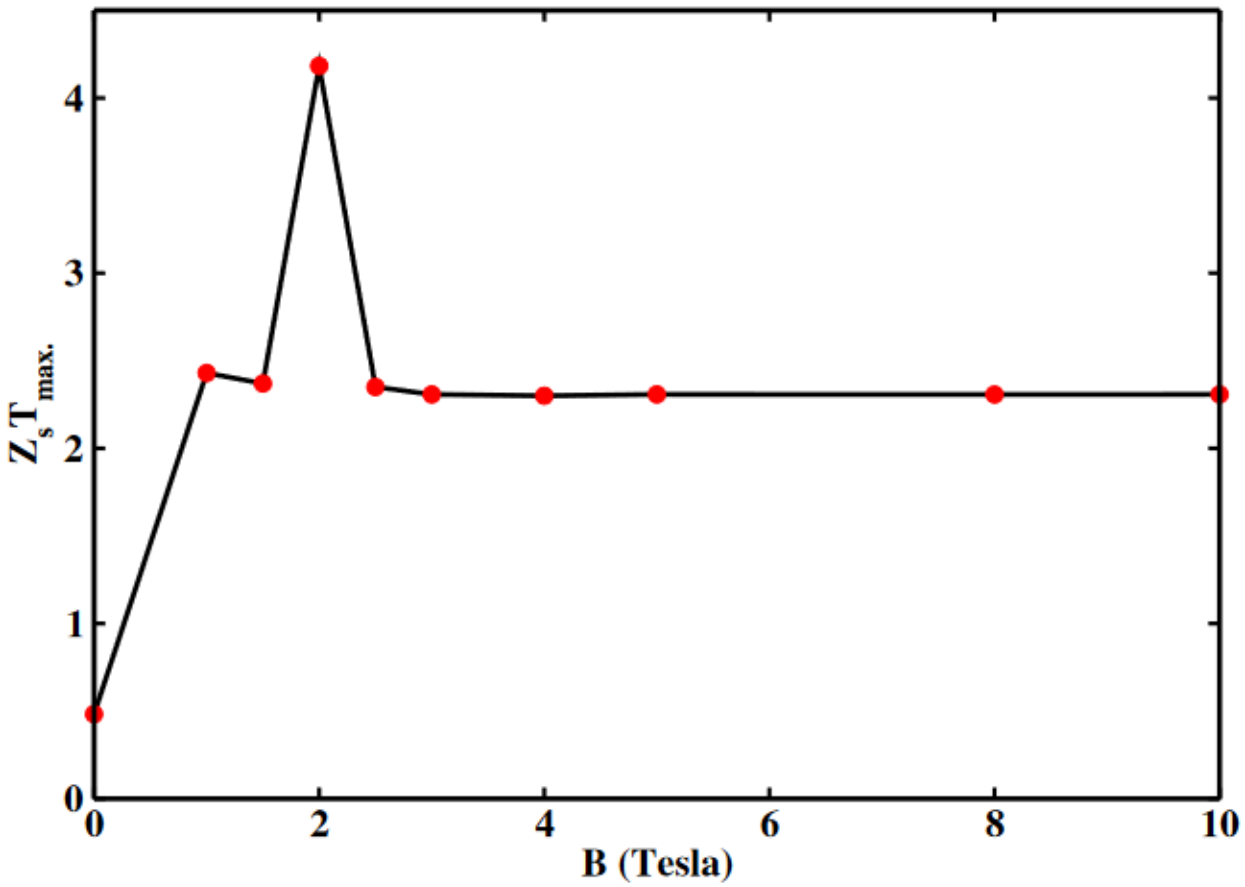

Figure S 7. The maximum value of Z_sT as a function of different magnetic field (B).