Electronic Supplementary Material (ESI) for Nanoscale.

High-performance thermoelectricity in edge-over-edge zinc-porphyrin molecular wires.

Supporting information

High-performance thermoelectricity in edge-over-edge zinc-porphyrin molecular wires.

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The wavefunction (φ) corresponding to the vibrational modes are the eigenvectors of the Dynamical Matrix D:

$$D\varphi = \omega^2\varphi \qquad (S1)$$

The weight P_i of the wavefunction (φ) of the degree of freedom (q') on each modes *i* can be calculated as:

$$P_i = \sum_{j \in q'} |\varphi_{ij}|^2 \qquad (S2)$$

The participation ratio of the modes associated with the center of mass motion on x = [1 0 0], y = [0 1 0] and z = [0 0 1] directions can be calculated as:

$$R = \sqrt{Q_{x'}^2 + Q_{y'}^2 + Q_{z'}^2} \qquad (S3)$$

where $Q_\beta = \langle \varphi \,|\, \beta \rangle / \sqrt{N}$ $(S4)$

and $\beta = x', y', z'$

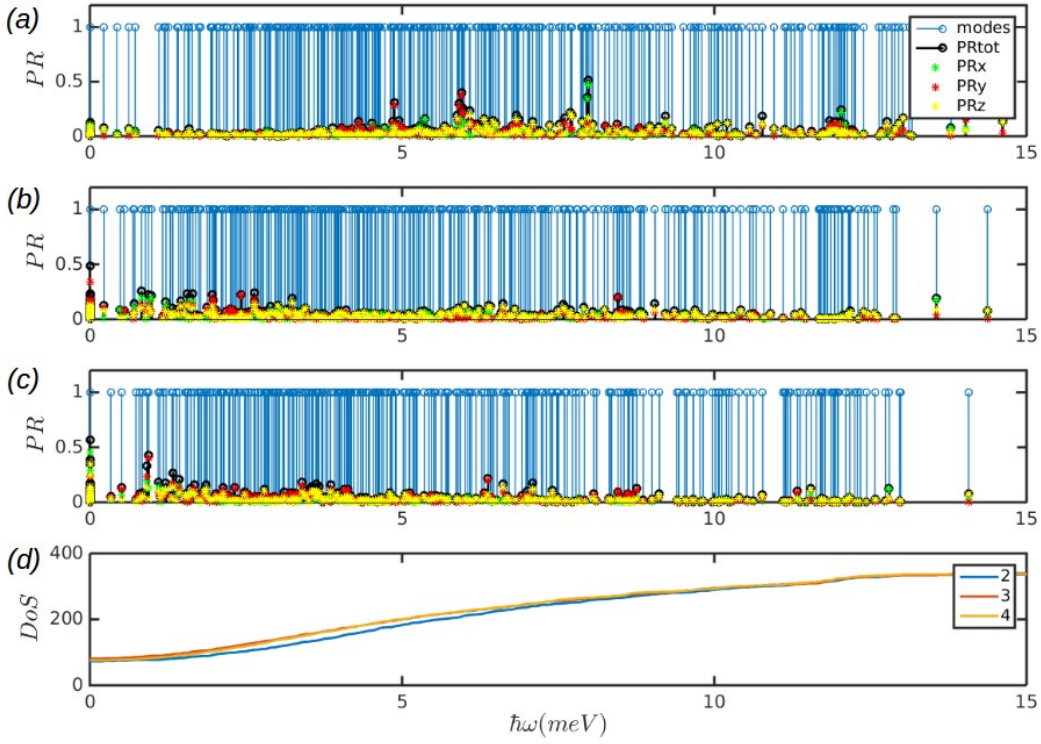

Figure S1. Participation ratio of the molecular cores consisting of the ZnP(s) and linkers on the modes associated with whole of the molecule attached to the surface of the gold electrodes. For the edge-over-edge structre (**2**), the modes has pushed to the higher energies and only in plane transverse modes are transmitted. Out-of plane transverse mode are suppressed due to the more rigid nature of (**2**) compared to (**3**) and (4) in out-of-plane transverse direction. (d) shows the density of modes for (**1-3**).

Structure	**Experimental Conductance**	**Theory Conductance**
Monomer (**1**)	$2.7\text{x}10^{-5}$	$1.09\text{x}10^{-1}$
Dimer (**3**)	$1.55\text{x}10^{-5}$	$6.35\text{x}10^{-2}$
Ratio (monomer/dimer)	1.74	1.72

Table.S1 The experimental and theoretical electrical conductance and their ratio for dimer and monomer.

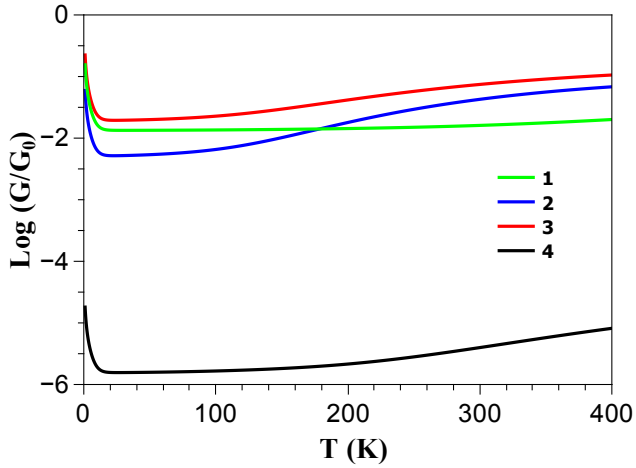

Figure S2. The electrical conductance as a function of temperature for ZnP monomer (**1**), edge-over-edge ZnP (**2**), ZnP connected through an oligoyne chain (**3**) and ZnP-dimer connected through pyridyl rings (**4**).

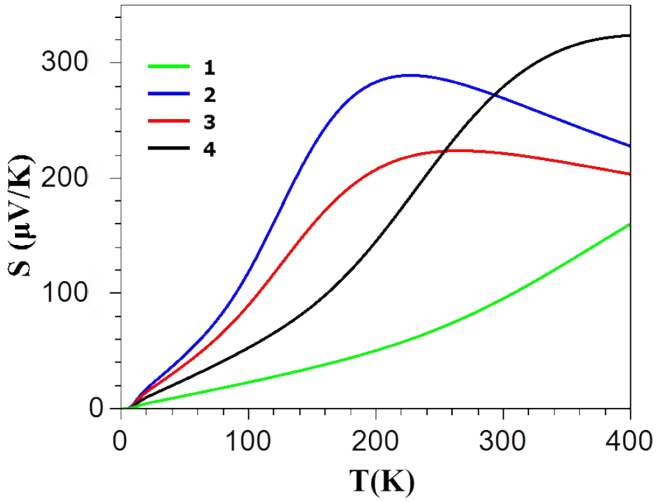

Figure S3. The Seebeck coefficient S as a function of temperature for ZnP monomer (**1**), edge-over-edge ZnP (**2**), ZnP connected through an oligoyne chain (**3**) and ZnP-dimer connected through pyridyl rings (**4**).