Nanoscale Advances

ARTICLE

Supporting Information

Radical Enhancement of Molecular Thermoelectric Efficiency

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Table S1. Spin orbitals of BPyNP radical

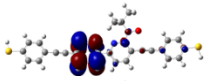
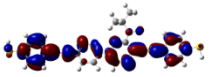
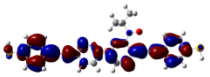
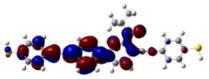
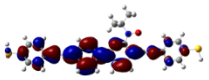
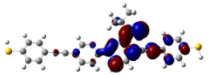
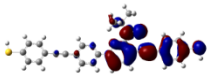
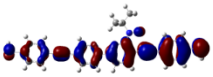
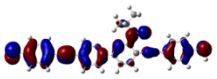
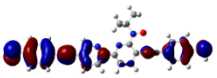
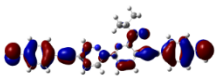
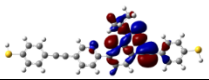
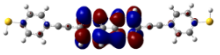
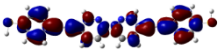
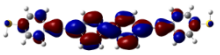
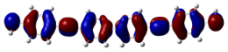
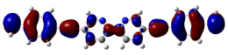
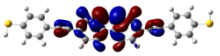
Level	spin	Energy (eV)	Spin orbitals of BPyNP radical
LUSO+2	α/↑	-1.28	
LUSO+2	β/↓	-1.54	
LUSO+1	α/↑	-1.57	
LUSO+1	β/↓	-2.37	
LUSO	α/↑	-2.48	
LUSO	β/↓	-2.73	
HOSO	α/↑	-5.44	
HOSO	β/↓	-5.92	
HOSO-1	α/↑	-6.17	
HOSO-1	β/↓	-6.26	
HOSO-2	α/↑	-6.29	
HOSO-2	β/↓	-6.67	

Table S2. Molecular orbitals of BPy

Level	Spin	Energy (eV)	Molecular orbitals of BPy
LUMO+2	↑↓	-1.17	
LUMO+1	↑↓	-1.63	
LUMO	↑↓	-2.36	
HOMO	↑↓	-5.98	
HOMO-1	↑↓	-6.26	
HOMO-2	↑↓	-6.91	

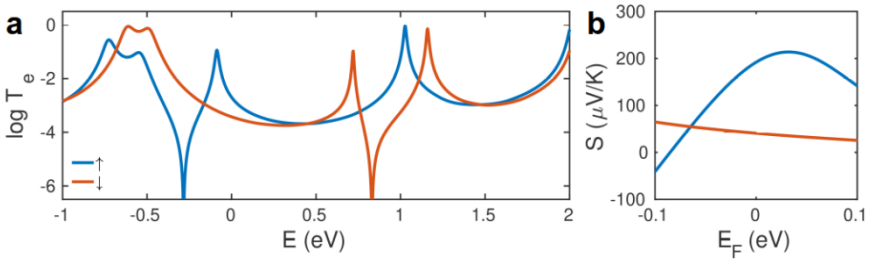


Fig. S1. (a) Transmission probability of electrons with different spin and energy *E* passing through BPyNO radical from one electrode to the other. (b) Room temperature Seebeck coefficient for majority and minority spins traversing through BPyNO radical versus electrodes Fermi energy.

Table S3. Total energy of BPyNO core in the different charge state. Adding an electron to this core is energetically easier than removing an electron from it.

Charge	0	-1	+1
Total Energy (eV)	-21293.38	-21294.64	-21286.14
Total Energy Differences (eV)	0	-1.26	7.24