Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Computational screening of structural and compositional factors for electrically conductive coordination polymers

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1. Computational details: plane wave cut-off

The plane-wave cut-off has been tested on Fe, which has the softness pseudo-potential amongst all of the atoms used (Figure S1). The convergence was set to an error smaller than 1% than the total energy in the complete basis set limit.

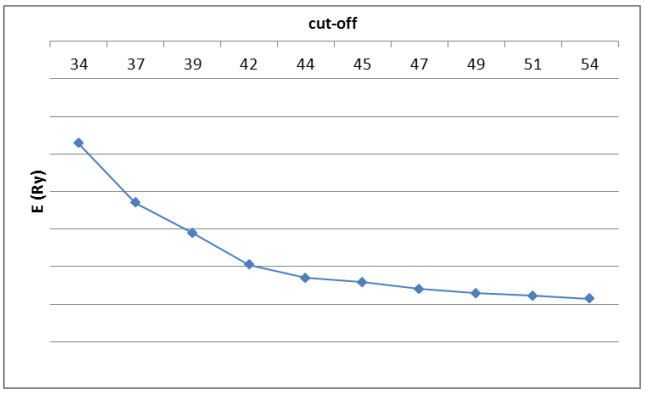

Figure S1. Example plane-wave cut-off convergence tests for Fe.

2. Computational details: equilibrium cell constants

Table S1 Optimised lattice parameters (Å) of the $Na_{2n}[Ni(C_xS_y)]_n$ compounds.

Organic Component	*r*	a	b	c
Ethylene	0	6.142	15.0	12.0
Benzene	1	8.625	15.0	12.0
Naphthalene	2	11.081	15.0	12.0
Anthracene	3	13.536	15.0	12.0
Tetracene	4	15.984	15.0	12.0
Pentacene	5	18.433	15.0	12.0
Naphthalene, side-on	2a	9.275	17.0	12.0
Pyrene	4a	11.131	17.0	12.0

Table S2 Optimised lattice parameters (Å) of r = 1 and 5 polymers with oxygen, S and Se bridging substituents $Na_{2n}[Ni(C_xS_y)]_n$ compounds.

Linker	Organic Ligand	a	b	c
O	Benzene	7.574	15.0	12.0
S	Benzene	8.625	15.0	12.0
Se	Benzene	9.015	15.0	12.0
O	Pentacene	17.372	15.0	12.0
S	Pentacene	18.433	15.0	12.0
Se	Pentacene	18.836	15.0	12.0

Table S3 Optimised lattice parameters (Å) for the Ni r = 1 polymer as a function of metal coordination environment and oxidation state.

Oxidation state	Coordination	a	b	c
Aromatic	Octahedral	9.046	16.0	15.0
Aromatic	Square planar	8.625	15.0	12.0
Quinoid	Square planar	8.412	15.0	12.0

Table S4 Optimised lattice parameters (Å) of prototype polymers examined. The corresponding structures are given in Figure S1.

Compound	Metal	Organic Ligand	a	b	c
I	Cu	TCNE	8.076	18.0	12.0
II	Cu	DCNQI	25.378	12.5	12.5
III	Ni	Pyrimidine	13.256	14.5	12.0
IV	Ag	Imidazole	12.503	18.0	12.0
V	Fe	Triazole	7.227	18.0	18.0
VI	Cr	Cyanide	11.685	14.0	14.0
VII	Mn	TTPT	19.429	20.0	20.0
VII	Zn	TTPT	19.430	20.0	20.0
VIII	Zn	Thiolate	6.491	20.0	20.0