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| Authors | Tiana, Davide;Hendon, Christopher H.;Walsh, Aron;Vaid, Thomas P. |
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SUPPORTING INFORMATION

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

Davide Tiana,^a Christopher H. Hendon,^a Aron Walsh,^{a,*} and Thomas P. Vaid^{b,*}

^a Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, UK.

^b Department of Chemistry, The University of Alabama, Tuscaloosa, Alabama 35487, USA.

*To whom correspondence should be addressed: a.walsh@bath.ac.uk, tpvaid@ua.edu

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.

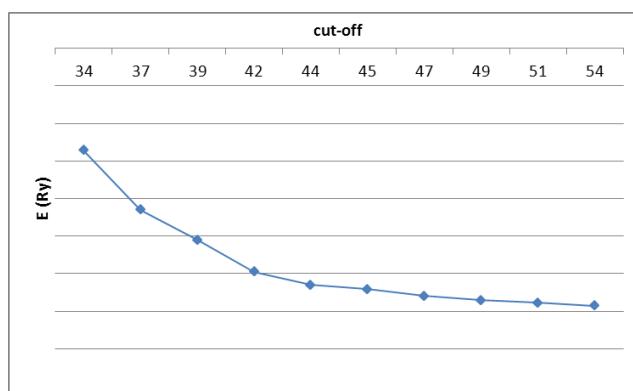


Figure S1. Example plane-wave cut-off convergence tests for Fe.

2. Computational details: equilibrium cell constants

Table S1 Optimised lattice parameters (\AA) of the $\text{Na}_{2n}[\text{Ni}(\text{C}_x\text{S}_y)]_n$ 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 (\AA) of $r = 1$ and 5 polymers with oxygen, S and Se bridging substituents $\text{Na}_{2n}[\text{Ni}(\text{C}_x\text{S}_y)]_n$ compounds.

| Linker | Organic Ligand | a | b | c |
|--------|----------------|--------|------|------|
| | | 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 (\AA) 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 (\AA) 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 |