Supplementary Information

Molecular-scale thermoelectricity: a worst-case scenario.

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1. Tight binding model

Supplementary Figure 1 shows two lattices, which are used to produce four examples of transmission curves shown in supplementary Fig 2.

**Supplementary Figure 1.** A structure formed by coupling left and right semi-infinite one-dimensional crystalline tight-binding (TB) chains (with sites energies $\varepsilon_0$ and nearest neighbour couplings $\gamma$ ) to (a): a scattering region with site energies $\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4$, and (b): As for (a), but with a pendant site of energy $\varepsilon_4$, attached to the chain by a coupling $\delta$. In each case, the left and right leads are coupled to the scattering region by weak couplings $\alpha$ and $\beta$.

**Supplementary Figure 2.** Transmission functions for symmetric examples of the structures in Fig. 1. (a): Transmission function of the tight-binding structure shown in Fig. 1a, obtained by choosing $\varepsilon_1=\varepsilon_2=\varepsilon_3=\varepsilon_4=0$, $\gamma=-1$ and $\alpha=\beta=-0.1$ For this choice of parameters, the junction is symmetric. (b): As for (a), but with a pendant site of energy $\varepsilon_4=0$ attached to the scatterer by a coupling $\delta=\alpha=\beta=-0.1$ (represented by bottom panel of Fig. 1). (c and d): As for (b), but $\varepsilon_4=-0.6$ and $+0.6$ respectively.
The above results correspond to symmetric junctions, for which $\beta=\alpha$. Next we study asymmetric junctions, for which $\beta\neq\alpha$, as shown in Supplementary Figure 3.

**Supplementary Figure 3.** Examples of transmission functions associated with asymmetric junctions, obtained from the structures of supplementary Fig. 2, but with $\beta\neq\alpha$ (i.e $\beta=-0.1$ and $\alpha=-0.2$).

The Seebeck coefficients corresponding to each transmission curve in Supplementary Figure 2, are shown in the bottom panel of Figure 3 of the main text, while those corresponding to Supplementary Figure 3 are shown in the bottom panel of Figure 4 of the main text.

The expression used for $S(E_F)$ is (see eg ref [34] of the main text)

$$S (T) = -\frac{1}{eT L_0}$$

where

$$L_i = \int dE (E - E_F)^i [-T(E) \frac{df(E)}{dE}]$$

In this equation, $e$ is the electronic charge and $f(E)$ is the Fermi function. This expression reduces to equation (1) of the main text, if $T(E)$ can be approximated by a straight line in a narrow energy range of order $k_B T$, centred on $E_F$; ie at a low enough temperature.
2. Molecules selected for study

Supplementary Figure 4: Structures of the molecules 1-17, 1-7 and 12, possess symmetric cores, whereas 8-11 and 13-17 possess asymmetric cores (Key: H = white, N = blue, O = red, S = yellow) studied in this work.
The ground state Hamiltonian and optimized geometry of each molecule was obtained using the density functional theory (DFT) code [41]. The local density approximation (LDA) exchange correlation functional was used along with double zeta polarized (DZP) basis sets and the norm conserving pseudo potentials. The real space grid was defined by a plane wave cut-off of 250 Ry. The geometry optimization was carried out to a force tolerance of 0.01 eV/Å. This process was repeated for a unit cell with the molecule between gold electrodes where the optimized distance between Au and the anchor group was obtained. From the ground state Hamiltonian, the transmission coefficient, the room temperature electrical conductance $G$ and Seebeck coefficient $S$ was obtained.

The above series of molecules were then connected to gold electrodes and the resulting junction geometries were relaxed. As examples, junctions formed from 3 and 6 are shown in Figure S5.

3. DFT results for the transmission functions and Seebeck coefficients of structures 1–17.

For each of the above molecules, Supplementary Figures 6-18 show the transmission coefficients as a function of electron energy $E$ and Seebeck coefficients $S$ evaluated at room temperature using equation S1 for various Fermi energies $E_F$, relative to the DFT-predicted Fermi energy $E_F^{DFT}$. 

Supplementary Figure 5: Optimised structures of 3 and 6 in Au|molecule|Au junctions.
Supplementary Figure 6: (Left panel). Transmission coefficient $T(E)$ for 1. 1a: The grey plot is obtained when the molecule is located symmetrically within the junction. 1b and 1c: The yellow and brown plots are obtained from slightly asymmetric junctions, in which the distance (or angle) to one electrode differs slightly from the other. (Right panel). Corresponding Seebeck coefficients $S(E_F)$ for junctions 1a-c. Note the negative yellow/brown area is much smaller than positive grey area for the asymmetric junctions 1b and 1c, which possess silent LUMOs. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.

Supplementary Figure 7: (Left panel). Transmission coefficient $T(E)$ for 2. 2a: The grey plot is obtained when the molecule is located symmetrically within the junction and the rotaxane ring is located at the centre of the oligoyne backbone. 2b and 2c: The yellow and brown plots are obtained from slightly asymmetric junctions, in which the rotaxane ring is closer to one end or other. (Right panel). Corresponding Seebeck coefficients $S(E_F)$ for junctions 2a-c. Note the negative yellow/brown area is much smaller than positive grey area for the asymmetric junctions 2b and 2c, which possess silent LUMOs. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.
**Supplementary Figure 8:** (Left panel). Transmission coefficient $T(E)$ for 3. 1a: The grey plot is obtained when the molecule is located symmetrically within the junction. 1b and 1c: The yellow and brown plots are obtained from slightly asymmetric junctions, in which the distance (or angle) to one electrode differs slightly from the other. (Right panel). Corresponding Seebeck coefficients $S(E)$ for junctions 1a-c. Note the negative yellow/brown area is much smaller than positive grey area for the asymmetric junctions 1b and 1c, which possess silent LUMOs. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.

**Supplementary Figure 9:** Transmission coefficient $T(E)$ for 4 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the positive grey area equals negative grey area due to symmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.
**Supplementary Figure 10:** Transmission coefficient $T(E)$ for 5 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the positive grey area equals negative grey area due to symmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.

**Supplementary Figure 11:** Transmission coefficient $T(E)$ for 6 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the positive grey area equals negative grey area due to symmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.
Supplementary Figure 12: Transmission coefficient $T(E)$ for 7 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the positive grey area equals negative grey area due to symmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.

Supplementary Figure 13: Transmission coefficient $T(E)$ for 8 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the negative yellow area is smaller than positive grey area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.
Supplementary Figure 14: Transmission coefficient $T(E)$ for 9 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the negative yellow area is smaller than positive grey area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.

Supplementary Figure 15: Transmission coefficient $T(E)$ for 10 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the negative yellow area is smaller than positive grey area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.
Supplementary Figure 16: Transmission coefficient $T(E)$ for 11 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the negative yellow area is much smaller than positive grey area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.

Supplementary Figure 17: Transmission coefficient $T(E)$ for 12 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the positive grey area equals negative grey area due to symmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.
**Supplementary Figure 18:** Transmission coefficient $T(E)$ for 13 **(Left panel)**. Seebeck coefficient $S$ of the same molecule **(Right panel)**. Note the negative yellow area is smaller than positive grey area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula eqn. 1 of the main text.

**Supplementary Figure 19:** Transmission coefficient $T(E)$ for 14 **(Left panel)**. Seebeck coefficient $S$ of the same molecule **(Right panel)**. Note the positive grey area is smaller than negative yellow area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula eqn. 1 of the main text.
Supplementary Figure 20: Transmission coefficient $T(E)$ for **15** (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the positive grey area is smaller than negative yellow area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.

Supplementary Figure 21: Transmission coefficient $T(E)$ for **16** (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the negative yellow area is slightly bigger than positive grey area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.
Supplementary Figure 22: Transmission coefficient $T(E)$ for 17 (Left panel). Seebeck coefficient $S$ of the same molecule (Right panel). Note the negative yellow/brown area is slightly bigger than positive grey area due to asymmetry. The black solid curves are plots of equation S1 (see section 1 above), whereas the red solid lines are obtained using the low-temperature formula equ. 1 of the main text.

4. Summary of Seebeck calculations

For each of the above molecules, Table S1, shows the average Seebeck coefficients and the values of $\delta_H$. We also show values of the following quantities, which capture different aspects of asymmetry $\Delta_H$, $S_H$ and $S_L$. These are defined by

$$\Delta_H = \frac{E_0 - E_H}{E_L - E_0}$$  \hspace{1cm} (S3)

$$\delta_H = \frac{T(E_H)}{T(E_H) + T(E_L)}$$  \hspace{1cm} (S4)

$$S_H = \frac{1}{E_0 - E_H} \int_{E_H}^{E_0} dE S(E) = \frac{A_H}{E_0 - E_H}$$  \hspace{1cm} (S5)

$$S_L = \frac{1}{E_L - E_0} \int_{E_0}^{E_L} dE S(E) = \frac{A_L}{E_L - E_0}$$  \hspace{1cm} (S6)

$$< S > = \frac{1}{\Delta} \int_{E_H}^{E_F} dE_F S(E_F) = \frac{A_H + A_L}{\Delta}$$  \hspace{1cm} (S7)

$\delta_H$ can be regarded as an alternative to $\Delta_H$ as an indicator of transmission-coefficient asymmetry. $S_H$ is the average of all Seebeck coefficients obtained for values of $E_F$ between the HOMO and $E_0$, whereas $S_L$ is the average of all Seebeck coefficients obtained for values of $E_F$ between the LUMO and $E_0$. 
Table S1. Seebeck results for each molecule (using equations S3-S7)

| M  | $S_H$ | $S_L$ | $\Delta_H$ | $\delta_H$ | $<S>$ | Note               |
|----|-------|-------|-------------|------------|-------|--------------------|
| 1a | 312.3 | -305.7| 0.508       | 0.5        | +6.0  | Symmetric molecule |
| 1b | 312.3 | -177.5| 0.29        | 0.99       | +122.7| Asymmetric molecule|
| 1c | 312.3 | -154.5| 0.18        | 0.999      | +143.7| Asymmetric molecule|
| 2a | 202.2 | -191.5| 0.42        | 0.50       | +7.8  | Symmetric molecule |
| 2b | 60.8  | -191.5| 0.41        | 0.0026     | -95.4 | Asymmetric molecule|
| 2c | 39.4  | -191.5| 0.44        | 0.00046    | -111.0| Asymmetric molecule|
| 3a | 83.7  | -90.0 | 0.95        | 0.50       | -9.5  | Symmetric molecule |
| 3b | 33.7  | -90.0 | 0.87        | 0.065      | -84.4 | Asymmetric molecule|
| 3c | 22.5  | -90.0 | 0.95        | 0.03       | -101.2| Asymmetric molecule|
| 4  | 198.2 | -191.5| 0.48        | 0.50       | +3.3  | Symmetric molecule |
| 5  | 179.6 | -164.2| 0.37        | 0.50       | +6.1  | Symmetric molecule |
| 6  | 91.5  | -120.14| 0.93  | 0.50       | -8.6  | Symmetric molecule |
| 7  | 117.5 | -94.2 | 0.25        | 0.50       | +6.7  | Symmetric molecule |
| 8  | 178.2 | -107.8| 0.57        | 0.97       | +42.3 | Asymmetric molecule|
| 9  | 240.7 | -131.6| 0.59        | 0.98       | +60.0 | Asymmetric molecule|
| 10 | 217.8 | -115.4| 0.77        | 0.985      | 37.6  | Asymmetric molecule|
| 11 | 118.8 | -23.5 | 0.48        | 0.99       | +35.1 | Asymmetric molecule|
| 12 | 137.2 | -121.4| 0.98        | 0.50       | +6.2  | Symmetric molecule |
| 13 | 161.8 | -25.8 | 0.47        | 0.99       | +54.4 | Asymmetric molecule|
| 14 | 26.5  | -177.0| 0.077       | 0.004      | -43.6 | Asymmetric molecule|
| 15 | 13.9  | -118.9| 0.52        | 0.002      | -35.7 | Asymmetric molecule|
| 16 | 45.4  | -72.2 | 0.84        | 0.178      | -16.8 | Asymmetric molecule|
| 17 | 67.0  | -87.6 | 0.87        | 0.04       | -23.6 | Asymmetric molecule|

* Grey indicates symmetric junctions and yellow indicates asymmetric junctions

Supplementary Figs. 23 and 24 show that $S_H \approx S_L$ for some molecules (grey-circles), whereas for other molecules $S_H > S_L$ or vice versa, yellow/brown-circles). $S_H \approx S_L$ for 1a, 2a, 3a, 4-9 and 12 whereas, $S_H > S_L$ or vice versa for the rest (1b, 1c, 2b, 2c, 3b, 3c, 8-11 and 13-17).
**Supplementary Figure 23:** Seebeck results of the molecules studied in this work, $S_H$ and $S_L$ as a function of $\Delta H$. (The grey circles correspond to the symmetric junctions, while the yellow/brown circles correspond to the asymmetric junctions)

**Supplementary Figure 24:** Seebeck results of the molecules studied in this work, $S_H$ and $S_L$ as a function of $\delta_H$. (The grey circles correspond to the symmetric junctions, while the yellow/brown circles correspond to the asymmetric junctions)
Supplementary Figure 25: The values for $<S>$ from Fig. 6 of the main text, but plotted against $\Delta_H$ instead of $\delta_H$.

Fig 6 of the main text shows that negative values of $<S>$ tend to arise when $\delta_H$ is small, whereas positive values of $<S>$ tend to arise when $\delta_H$ is close to unity. In other words, the value of $<S>$ tends to be correlated with $\delta_H$. Fig 25 shows that there is no such clear correlation with $\Delta_H$.

5. Wave function plots for isolated molecules with their optimised geometries

The plots below (Supplementary Figures 26-43) show isosurfaces of the HOMO, LUMO, HOMO-1 and LUMO+1 of isolated molecules of 1-17.

Supplementary Figure 26: Wave function for 1. Top panel: Fully optimised geometry of 1. Lower panel: HOMO, LUMO along with their energies.
Supplementary Figure 27: Wave function for 2a. **Top panel:** Fully optimised geometry of 2a. **Lower panel:** HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies (2a, the case when the rotaxane ring is in the centre of the OPE backbone).

Supplementary Figure 28: Wave function for 2b (2c). **Top panel:** Fully optimised geometry of 2b (2c). **Lower panel:** HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies (2b and 2c)
have the same wave function, 2b when the rotaxane ring is close to the left end whereas 2c when the ring is close to the right end).

Supplementary Figure 29: Wave function for 3. Top panel: Fully optimised geometry of 3. Lower panel: HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies (3a, 3b and 3c have the same wave function).

Supplementary Figure 30: Wave function for 4. Top panel: Fully optimised geometry of 4. Lower panel: HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.
Supplementary Figure 31: Wave function for 5. Top panel: Fully optimised geometry of 5. Lower panel: HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.

Supplementary Figure 32: Wave function for 6. Top panel: Fully optimised geometry of 6. Lower panel: HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.
**Supplementary Figure 33:** Wave function for 7. **Top panel:** Fully optimised geometry of 7. **Lower panel:** HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.

Supplementary Figure 34: Wave function for 8. **Top panel:** Fully optimised geometry of 8. **Lower panel:** HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.
Supplementary Figure 35: Wave function for 9. Top panel: Fully optimised geometry of 9. Lower panel: HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.

Supplementary Figure 36: Wave function for 10. Top panel: Fully optimised geometry of 10. Lower panel: HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.
Supplementary Figure 37: Wave function for 11. Top panel: Fully optimised geometry of 11. Lower panel: HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.

Supplementary Figure 38: Wave function for 12. Top panel: Fully optimised geometry of 12. Lower panel: HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.
**Supplementary Figure 39:** Wave function for 13. **Top panel:** Fully optimised geometry of 13. **Lower panel:** HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.

\[ E_F = -3.28 \text{ eV} \]

HOMO: E = -5.31 eV
LUMO: E = -2.65 eV
HOMO-1: E = -5.57 eV
LUMO+1: E = -1.78 eV

**Supplementary Figure 40:** Wave function for 14. **Top panel:** Fully optimised geometry of 14. **Lower panel:** HOMO, LUMO, HOMO-1 and LUMO+1 along with their energies.

\[ E_F = -2.574 \text{ eV} \]

HOMO: E = -4.95 eV
LUMO: E = -1.52 eV
**Supplementary Figure 41:** Wave function for 15. **Top panel:** Fully optimised geometry of 15. **Lower panel:** HOMO, LUMO along with their energies.

**Supplementary Figure 42:** Wave function for 16. **Top panel:** Fully optimised geometry of 16. **Lower panel:** HOMO, LUMO along with their energies.
Supplementary Figure 43: Wave function for 17. **Top panel:** Fully optimised geometry of 17. **Lower panel:** HOMO, LUMO along with their energies.

6. Result for alternative distributions of the Fermi energy

So far, we have considered only a worst-case scenario, in which the Fermi energy is uniformly distributed between the HOMO and LUMO energies $E_H$ and $E_L$ and asymmetries are needed to create a non-zero $< S >$. There are of course an infinite number of possible Fermi-level distributions $P(E_F)$, ranging from the above worst-case scenario to the opposite extreme, in which there are no fluctuations and $E_F$ adopts a definite value. In the latter case, $S(E_F)$ can be read off from curves such as those in the lower panels of Figs. 3 and 4 of the main text. As intermediate cases, we consider the case where $E_F$ is uniformly distributed between energies $E_a$ and $E_b$, where $E_a = E_H + x \left( \frac{E_L - E_H}{2} \right)$, $E_b = E_L - x \left( \frac{E_L - E_H}{2} \right)$. If the parameter $x = 0$, then this corresponds to the worst-case scenario, whereas if $x = 1$, $E_a = E_b = (E_H + E_L)/2$ and $E_F$ is confined to the middle of the HOMO-LUMO gap, with no fluctuations. In what follows, we show results not only for the average single-molecule Seebeck coefficient, defined by

$$< S_{\text{single}} > = \frac{1}{E_a - E_b} \int_{E_a}^{E_b} dE_F \, S(E_F) \tag{S8}$$

But also we show results for conductance-weighted Seebeck coefficient, defined by

$$< S_{\text{SAM}} > = \frac{< S_G >}{< G >} \tag{S9}$$

where

$$< S_G > = \frac{1}{E_a - E_b} \int_{E_a}^{E_b} dE_F \, S(E_F) \, T(E_F) \quad \text{and} \quad < G > = \frac{1}{E_a - E_b} \int_{E_a}^{E_b} dE_F \, T(E_F) \tag{S10}$$

As discussed in ref [34] of the main text, $< S_{\text{SAM}} >$ is the average Seebeck coeffient of a self-assembled monolayer (SAM) of a parallel array of non-interacting molecules, whose Fermi energies are uniformly distributed between energies $E_a$ and $E_b$. For the 17 molecules considered here, Figure S44
shows plots of $<S_{\text{single}}>$ and $<S_{\text{SAM}}>$ for various values of $x$. Interestingly, the molecules 1b, 2b, 3b, 1c, 2c, 3c with silent orbitals deliver large Seebeck coefficients, which are relatively insensitive to the value of $x$, which shows that these molecules are advantageous for thermoelectricity. These distributions are unbiased, in the sense that they are symmetric about the gap centre. Clearly the thermoelectric performance of these molecules could be improved by biasing the distributions of $E_F$ with a judicious choice of anchor group. If the worst-case-scenario value of $<S>$ is negative, then this could be improved by utilising pyridyl anchors, which bias $E_F$ towards the LUMO, whereas if the worst-case-scenario value of $<S>$ is positive, then this could be improved by utilising thiol anchors, which bias $E_F$ towards the HOMO.
7. Power factor

Figure S45 shows the power factor \( <S_G^2>/ <G> \) plotted against \( x \) for both symmetric and asymmetric molecules. It demonstrates that symmetric molecules have quite low power factors (grey circles), whereas asymmetric molecules have higher power factor and the asymmetric junctions containing molecules with silent orbitals consistently deliver high values.
Figure S45. DFT results for power factor $\langle S_G \rangle^2 / \langle G \rangle$ plotted against $x$, (The grey circles for symmetric junctions and coloured circles asymmetric junctions.)