WP5 – Organic heterointerfaces for efficient large-area thermoelectrics

- Recent renewed interest in solar thermoelectric generators (STEGs): With $ZT \approx 1$ efficiencies on the order of 5-7% achievable

Kraemer et al., Nat. Mat. 10, 532 (2011)

- Need for high performance large-area materials - Focus on conjugated polymer – carbon nanotube composites

- Key challenges:
  - Control of morphology
  - Doping
  - Transport across polymer / CNT interfaces
WP 5 - Partner contributions

- Hofmann (CAM-Eng) – CNT growth/synthesis
- Kar-Narayan (CAM-Mat) – Composite processing
- Nielsen (QMU) – Doping / conjugated polymer materials
- Baxendale, Reece, Fenwick, Bilotti (QMU) – Thermoelectric properties
- Bronstein (UCL-Chem) – Conjugated polymers
- Sirringhaus (CAM-Phys) – Thermoelectric properties, device physics
Challenge of maximising thermoelectric figure of merit

\[ ZT = \frac{S^2 \sigma T}{\kappa} \]

\[ S = \frac{1}{\sigma} \left( \frac{k_B}{e} \right) \int \left( \frac{E - E_F}{k_B T} \right) \sigma_E \left( -\frac{\partial f}{\partial E} \right) dE \]

\[ \sigma = \int \sigma_E \left( -\frac{\partial f}{\partial E} \right) dE \]

Wiedemann-Franz relationship: \[ \frac{\kappa_e}{\sigma} = LT \]

Performance of organic thermoelectric materials
High power factors in conjugated polymer / CNT layer-by-layer composites

Conjugated polymer wrapped, size-selected, single-wall CNT networks

• Doped with triethyloxoanion hexachloroantimonate
  \[(\text{CH}_3\text{CH}_2)_3\text{O}^+\text{SbCl}_6^-\]
High mobility conjugated polymers with low degree of energetic disorder

Low Urbach energy

High Seebeck, temperature-independent Seebeck

Torsion free backbone conformation

High mobility of 1.5-2.5 cm$^2$/Vs

Method for bulk chemical doping without disruption of ordered polymer microstructure

- Films retain high degree of order - F4-TCNQ intercalates into side chain layers – equivalent to modulation doping
- High conductivity up to 250 S/cm and relatively high power factors

Kang et al., Nat. Mat. 15, 896 (2016)