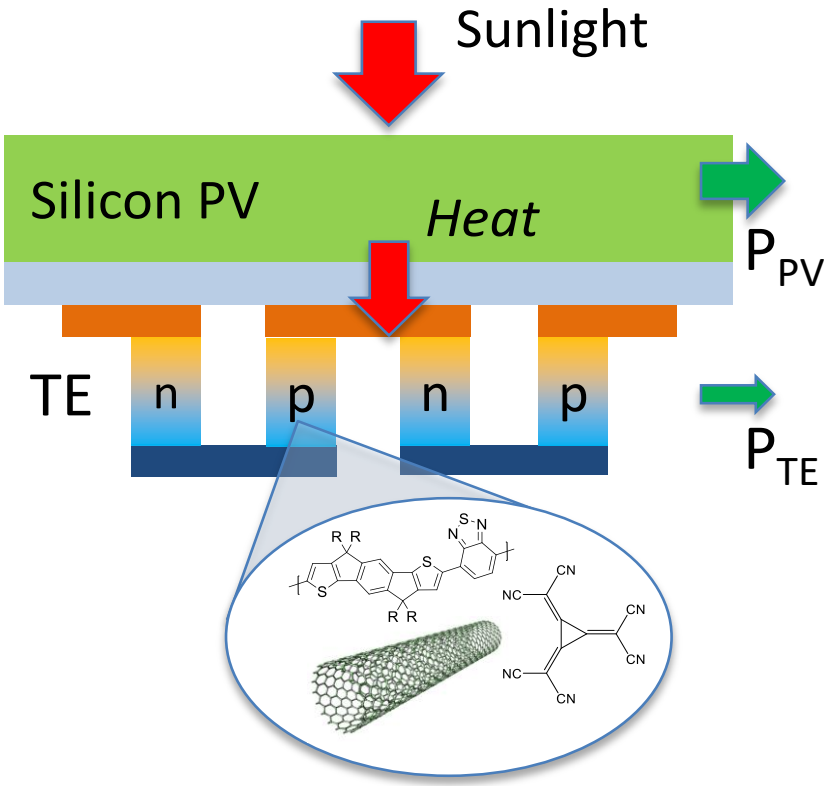
WP5 – Organic heterointerfaces for efficient large-area thermoelectrics



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

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

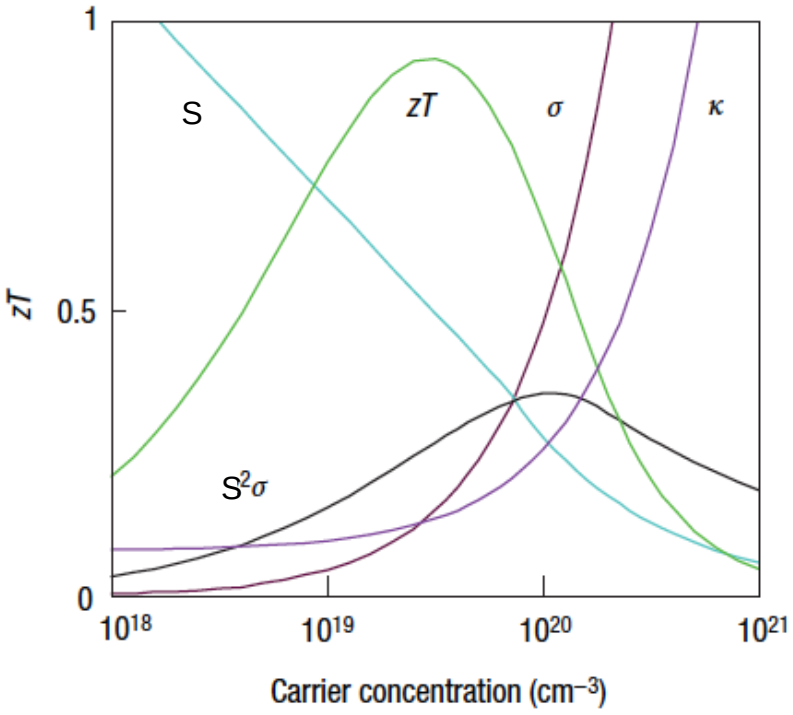
- Need for high performance large-are materials - Focus on conjugated polymer – carbon nanotube composites

- 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



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

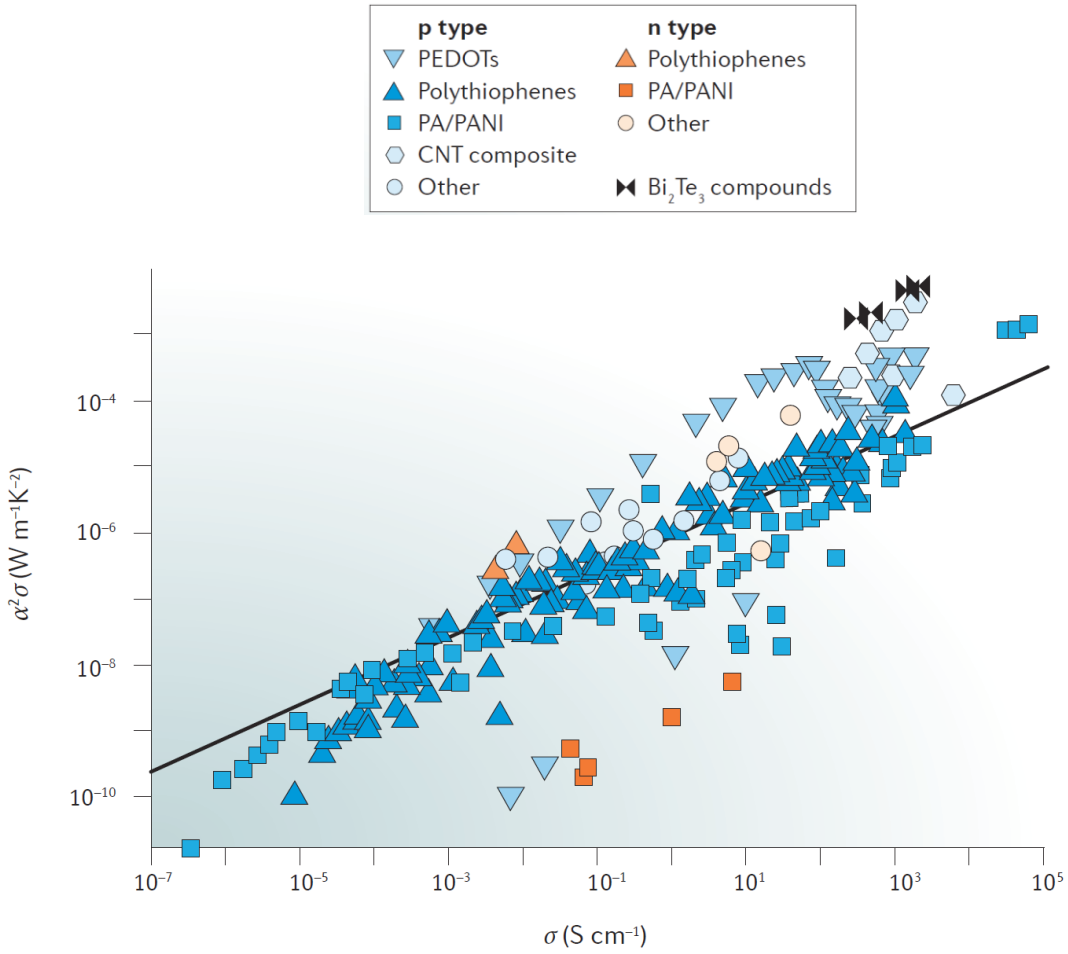
$$S = \frac{1}{\sigma}\left(\frac{k_B}{e}\right)\int\left(\frac{E - E_F}{k_B T}\right)\sigma_E\left(-\frac{\partial f}{\partial E}\right)dE$$

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

Wiedemann-Franz relationship: $\frac{\kappa_e}{\sigma} = LT$?

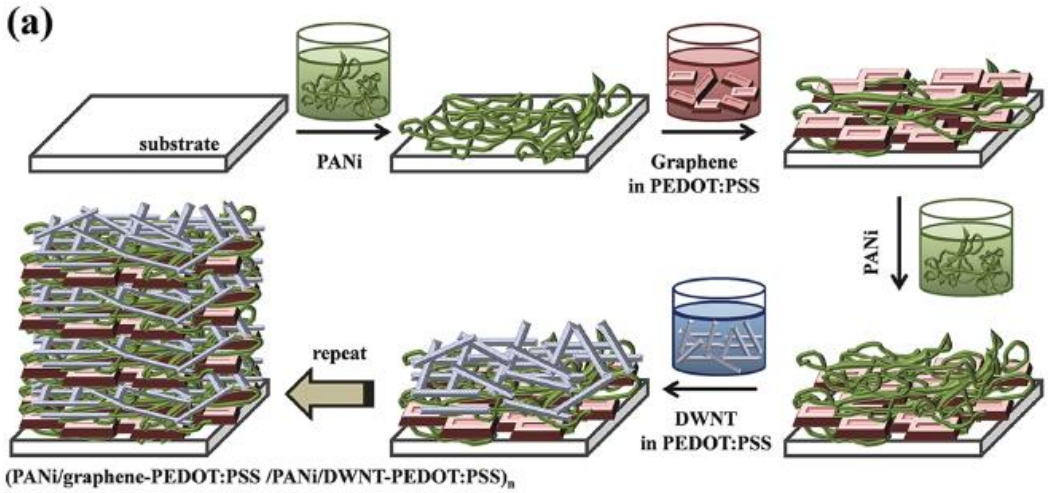
Snyder, G. J, and Toberer, E, S., Nature Materials **2008, 7**

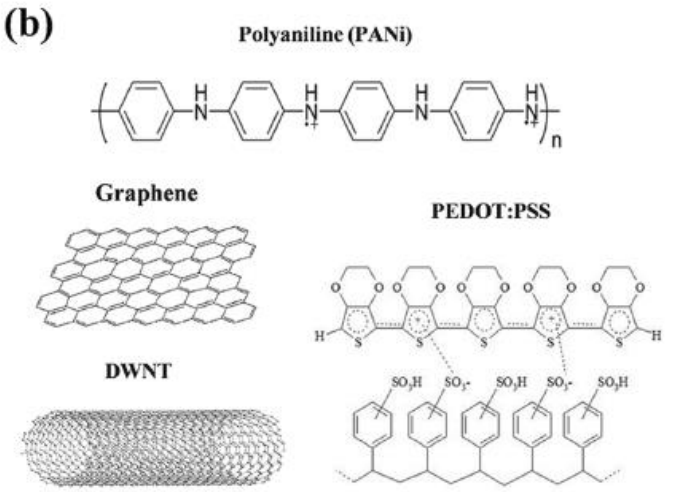
Performance of organic thermoelectric materials

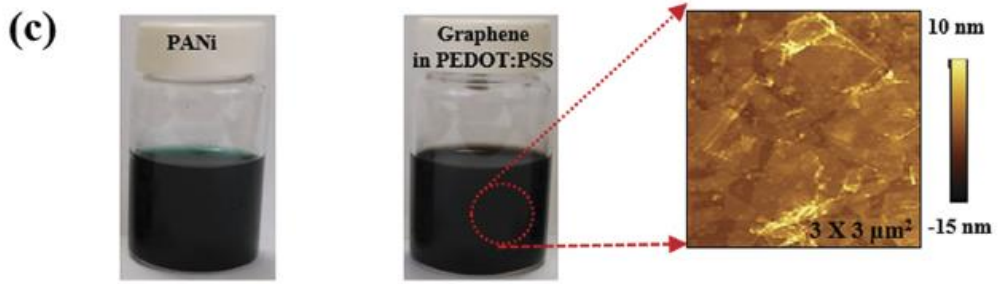


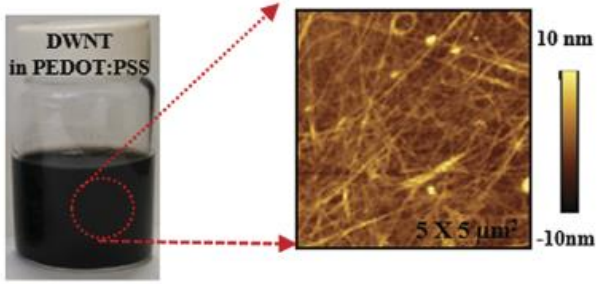
Glaudell, et. al, Adv. Energy. Mat, 2015, 5

High power factors in conjugated polymer / CNT layer-by-layer composites



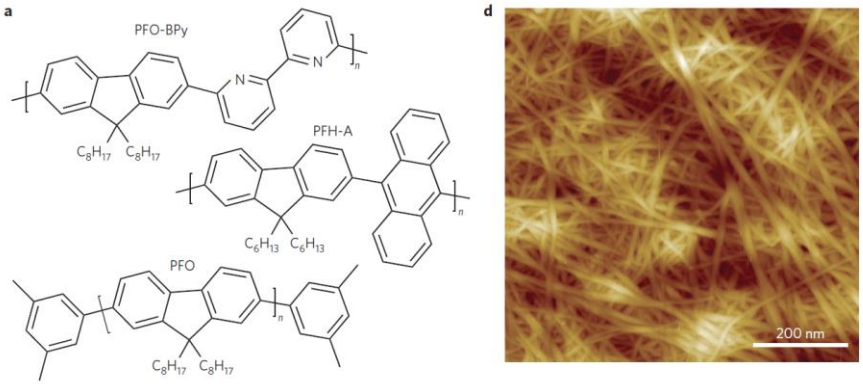


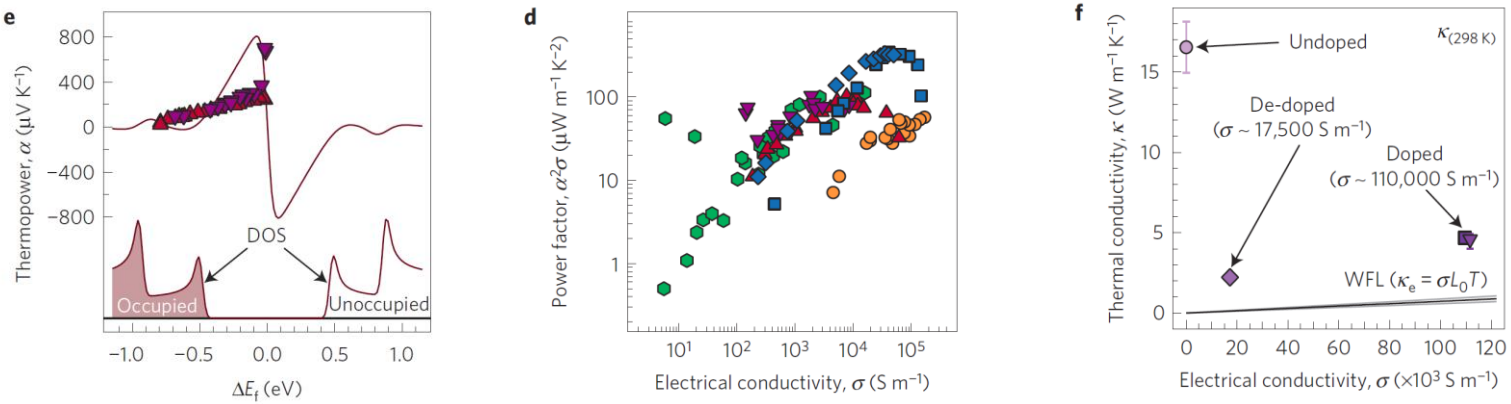




Cho et al., Adv. Energy Mater. 2016, 1502168

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

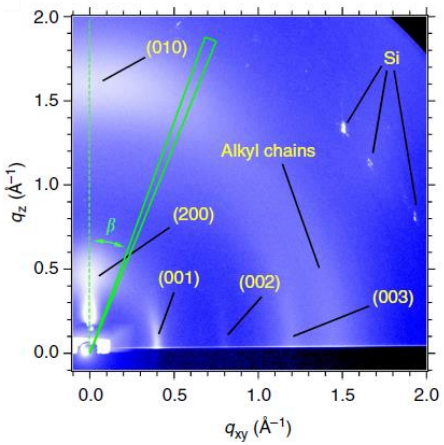




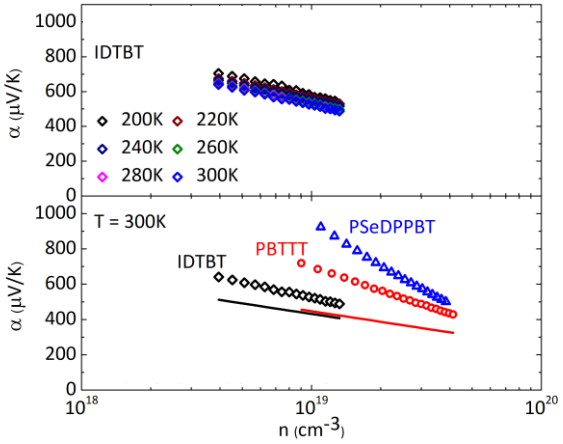
- Doped with triethyloxonium hexachloroantimonate $(CH_3CH_2)_3O^+$ $SbCl_6^-$

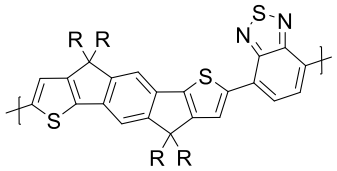
Ferguson et al., Nat. Energy 1, 16033 (2016)

High mobility conjugated polymers with low degree of energetic disorder

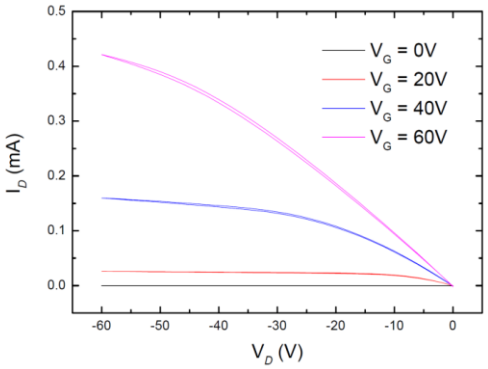


High Seebeck, temperature-independent Seebeck

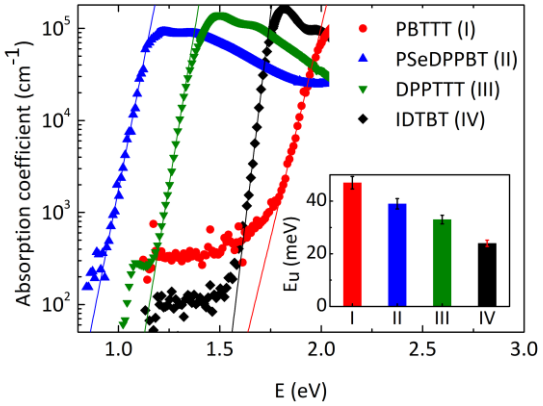




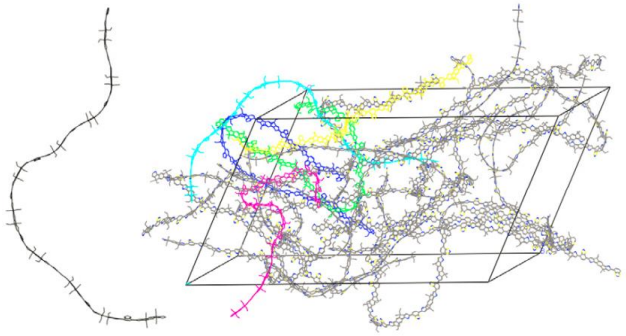
High mobility of 1.5- 2.5 cm^2/Vs



Low Urbach energy

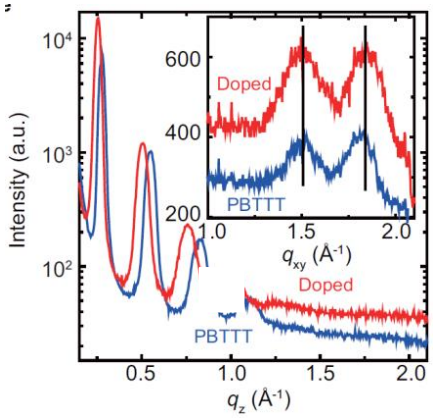


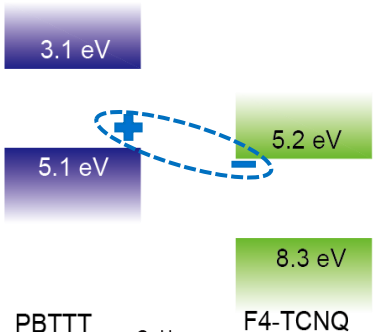
Torsion free backbone conformation



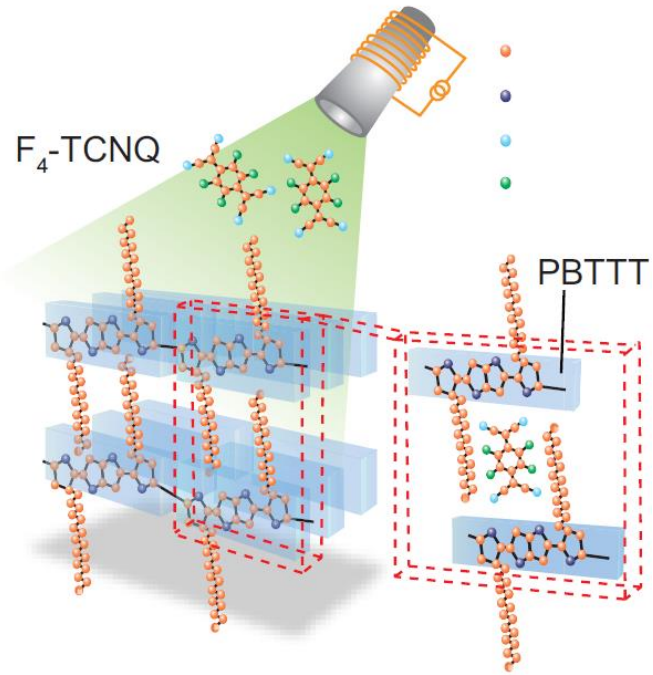
Venkateshvaran, Nikolka *et al.* Nature 515, 384 (2014)

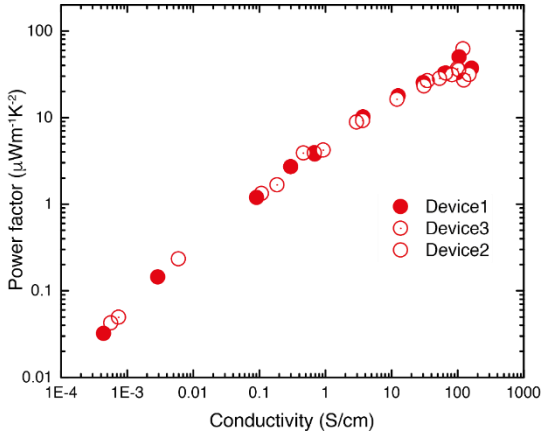
Method for bulk chemical doping without disruption of ordered polymer microstructure

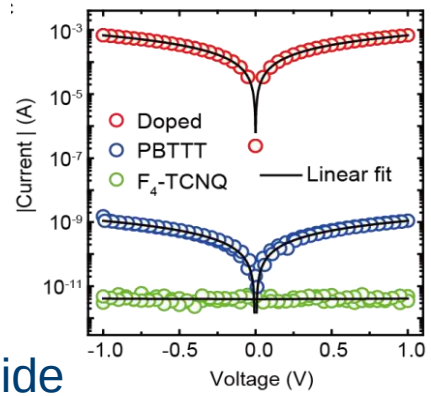




Doping by solid state diffusion







- 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)
Kang, et al., in preparation (2017)