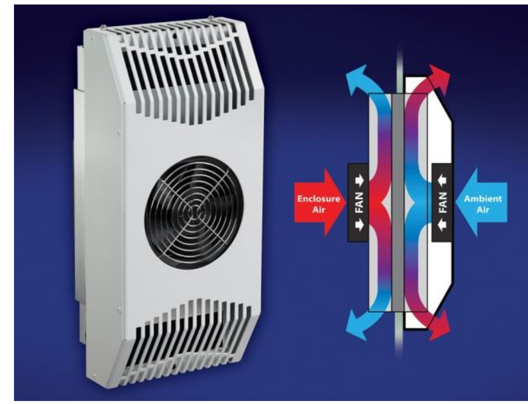
Thermoelectric Materials for Power Generation

Maryana Asaad

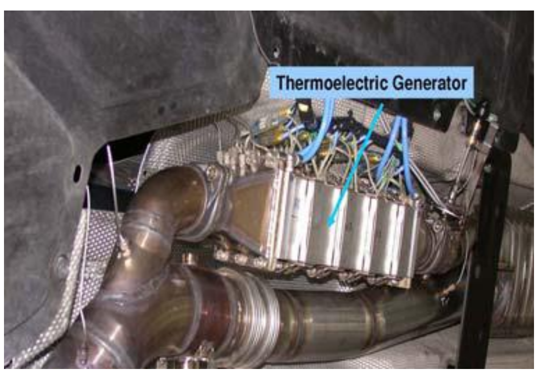
Introduction

Thermoelectricity involves the direct conversion between thermal and electrical energy

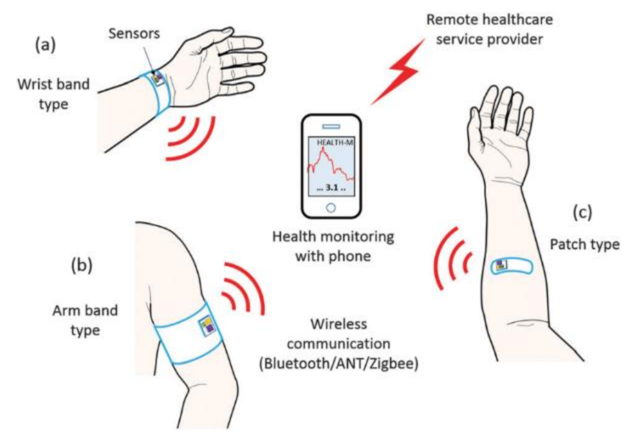
www.science.nasa.gov



www.mcleancoolingtech.com



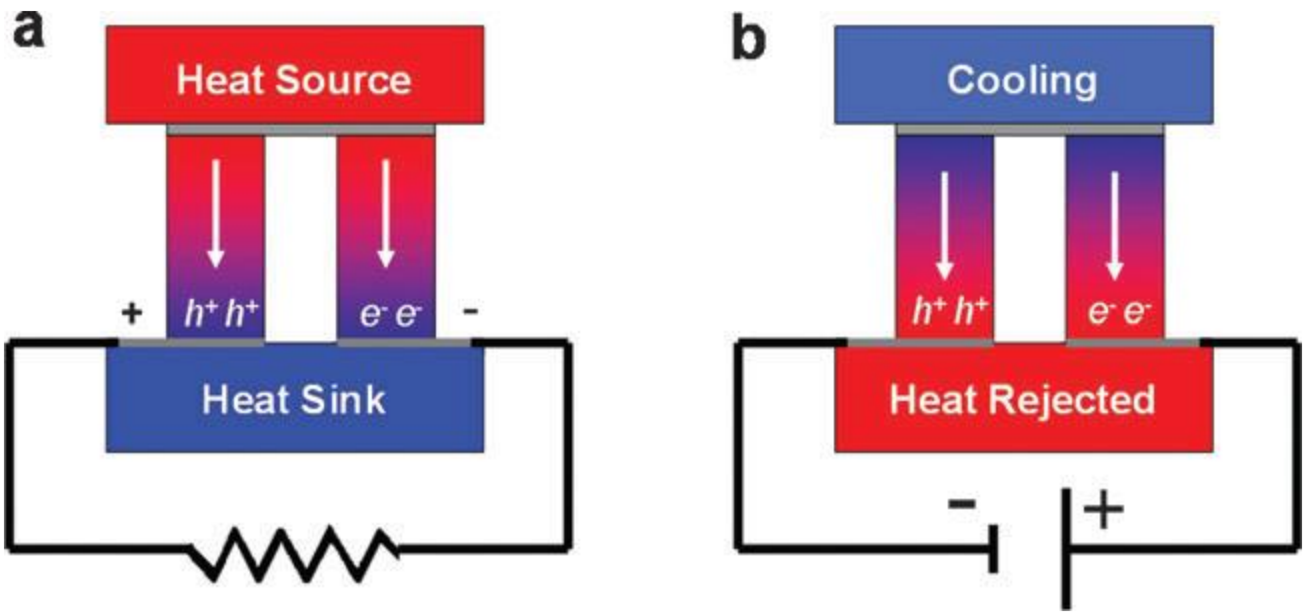
www.eere.energy.gov



*J.-H. Bahk et al.J.Mater.Chem.**2015**,3,10362*

Introduction

Thermoelectric devices: p-type and n-type semiconducting materials



A schematic of thermoelectric couples

R. B. Kaner et al.*Chem.Commun.,***2010**,46,8

Introduction

The efficiency of a thermoelectric material is defined by the figure of merit ZT:

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

$$\kappa = \kappa_{lat} + L\sigma T$$

S = Seebeck coefficient / V K^{-1}

σ = electrical conductivity / Ω^{-1} m^{-1}

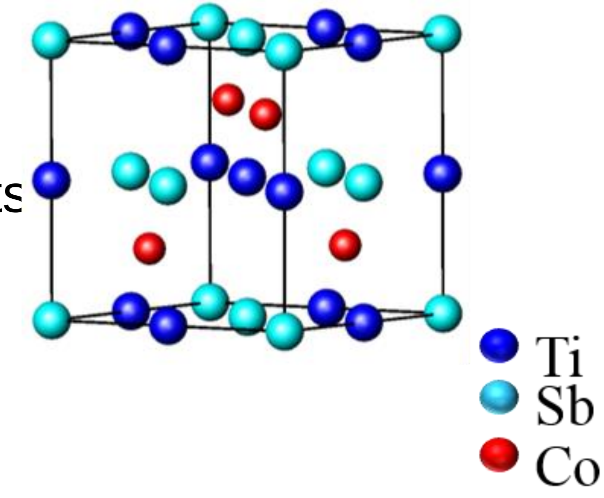
κ = Thermal conductivity / Wm^{-1} K^{-1}

M. S. Dresselhaus et al .*Energy.Environ.,* **2009**,2,46

Half Heusler Thermoelectric

Half-Heuslers

- General formula XYZ
- Semiconducting, 18 valence electrons
- Relatively non-toxic and earth abundant elements
- N-type :XNiSn, ZT = 1
- P-type : XCoSb, ZT = 0.5
- Large power factor: S^2/ρ = 4-6 $mWm^{-1}K^{-2}$
- Reasonably low thermal conductivity



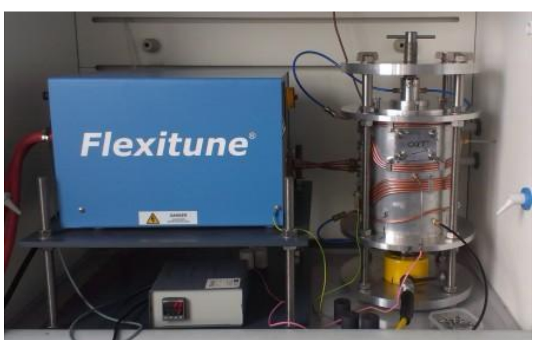
$$ZT = \frac{S^2 \boldsymbol{\sigma}}{\kappa} T$$

Synthesis and Characterisation

Synthesis

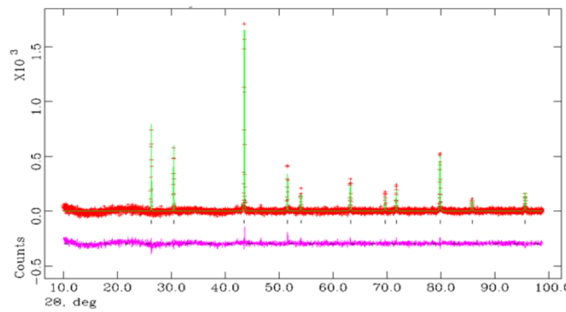
- Solid state reaction

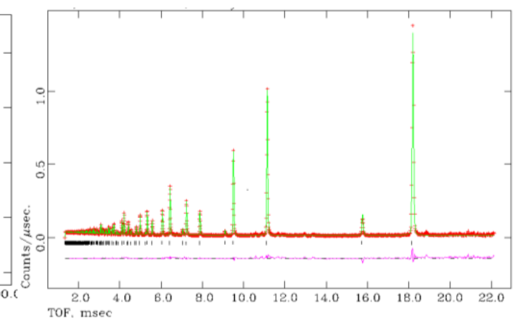

- Hot press



Characterisation

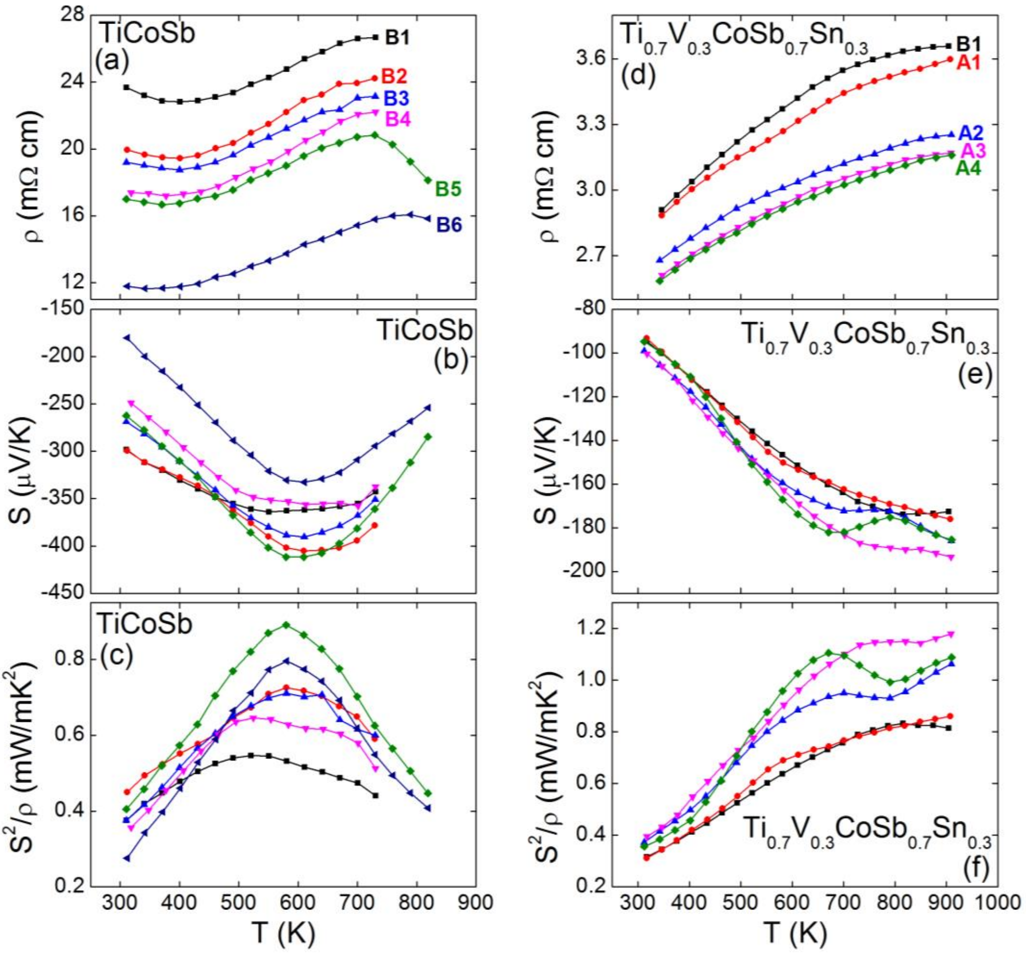
- Neutron/X-ray powder diffraction and Rietveld analysis

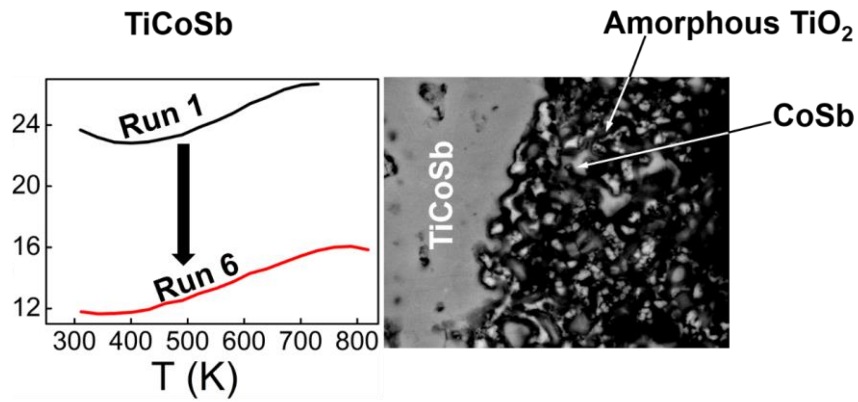




- Thermoelectric properties


High-Temperature Stability of TiCoSb-Based Compounds

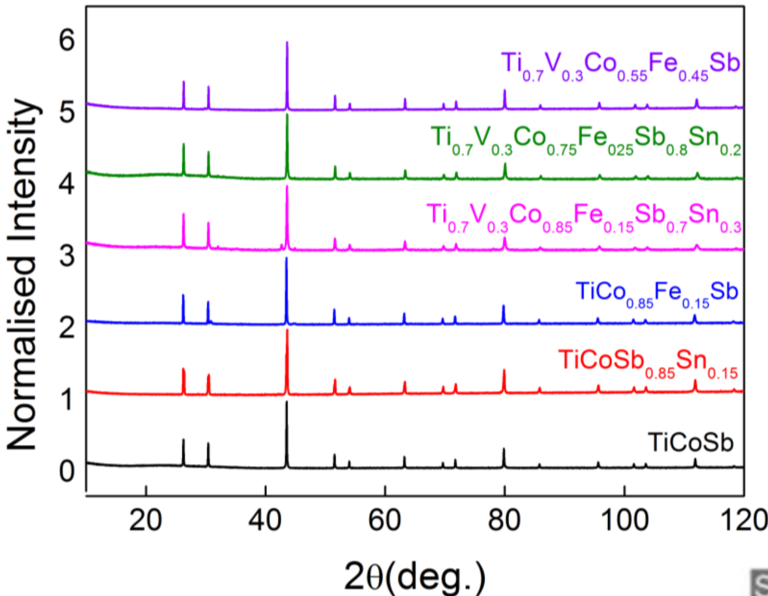


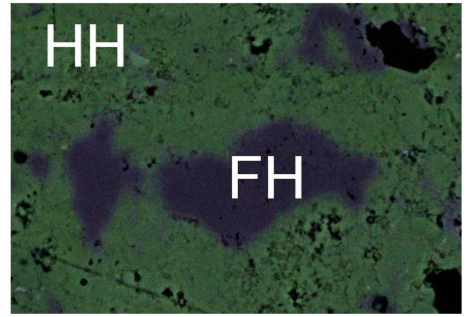


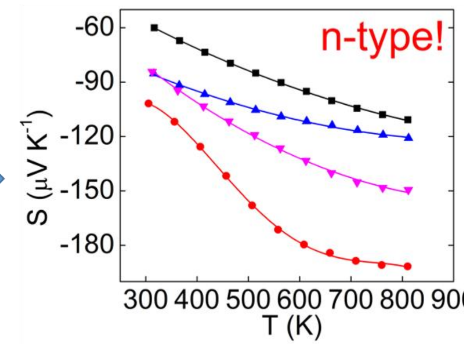
- TiCoSb not stable above 723K
- V,Sn doped sample appears more stable, but degradation evident in PXRD

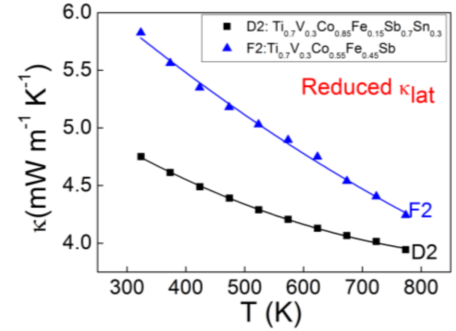
M. Asaad et al. RSC Adv., **2016**, *6*, 56511313

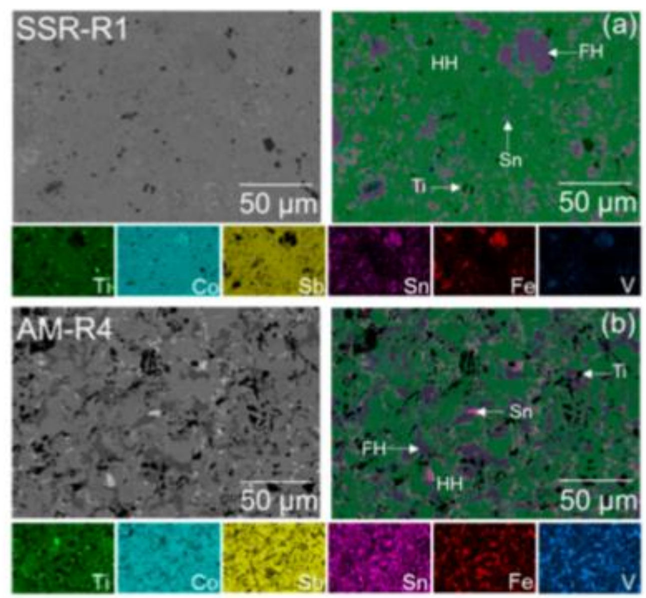
Unexpected N-Type Conduction in Half-Heuslers









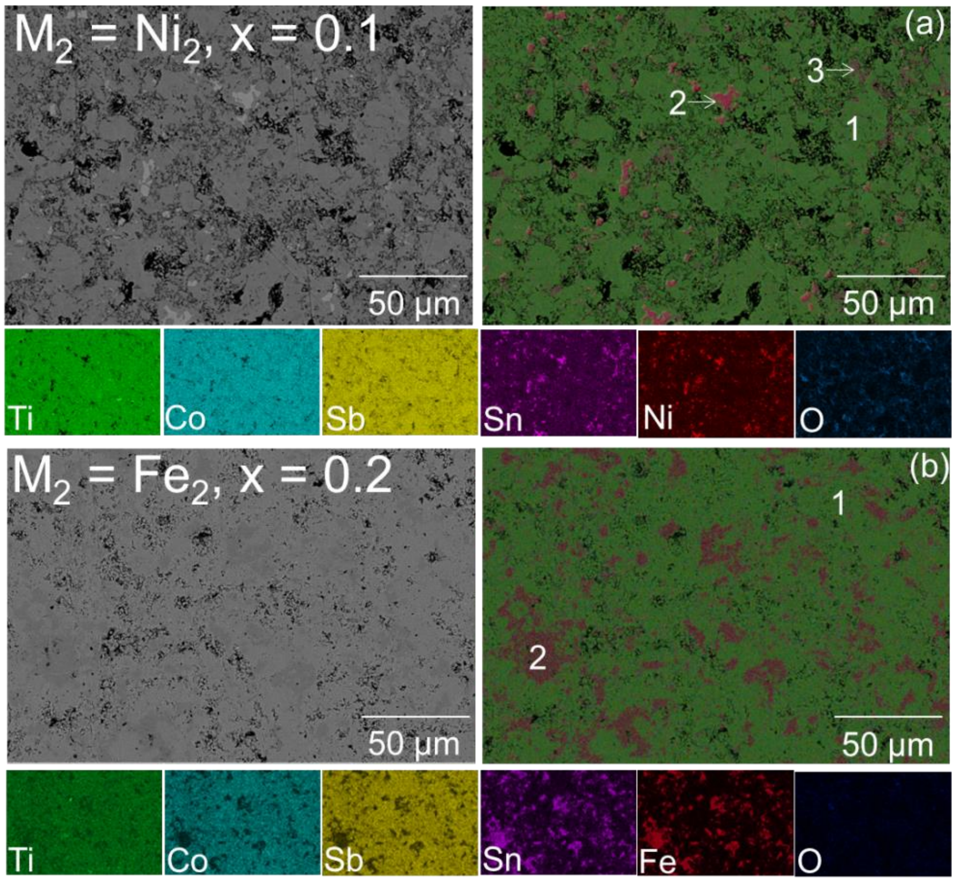


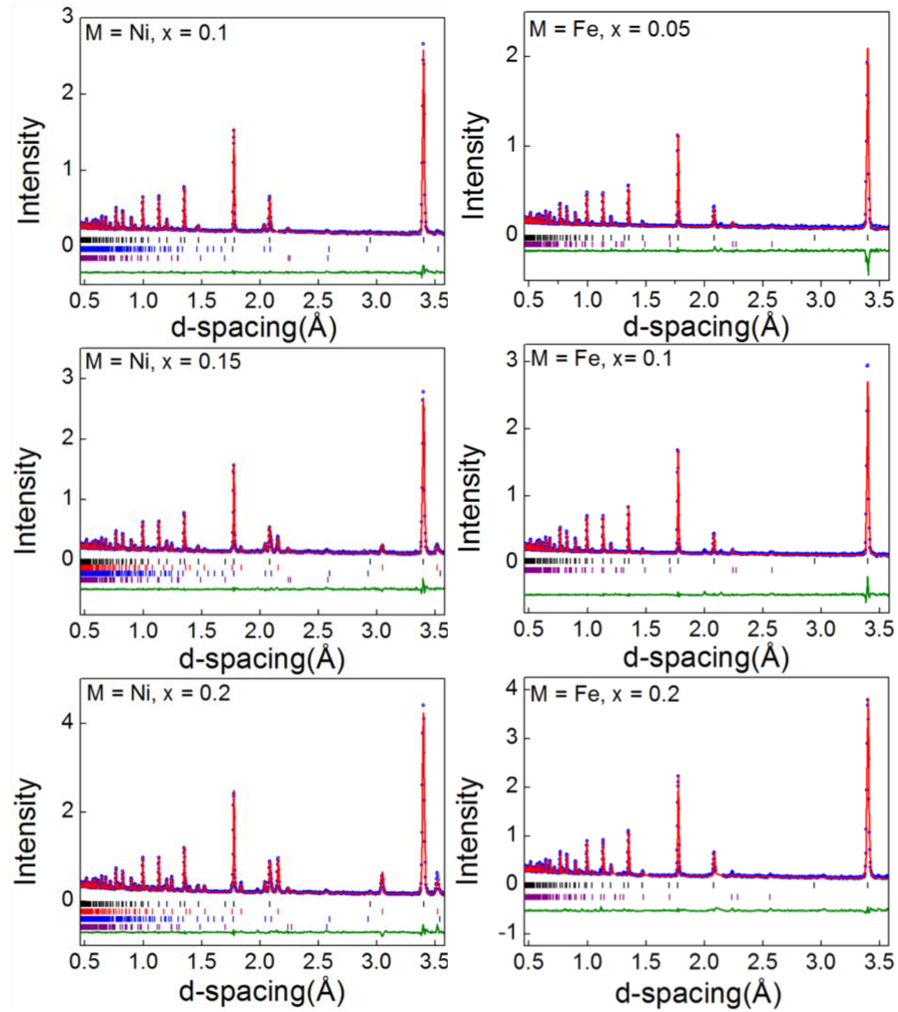
Phase segregation into 18+ VE half Heusler and V(Co,Fe)$_2$Sn FH phase

M. Asaad et al. Metals.,**2018**,*8*(11),935313

Half Heusler-Full Heusler composites

TiCoSb-TiM_2Sn (M= Ni, Fe) composites were investigated





M. Asaad et al. J. Solid State Chem.,**2019**,*276*,181-18913

National Graphene Institute

MANCHESTER 1824
The University of Manchester

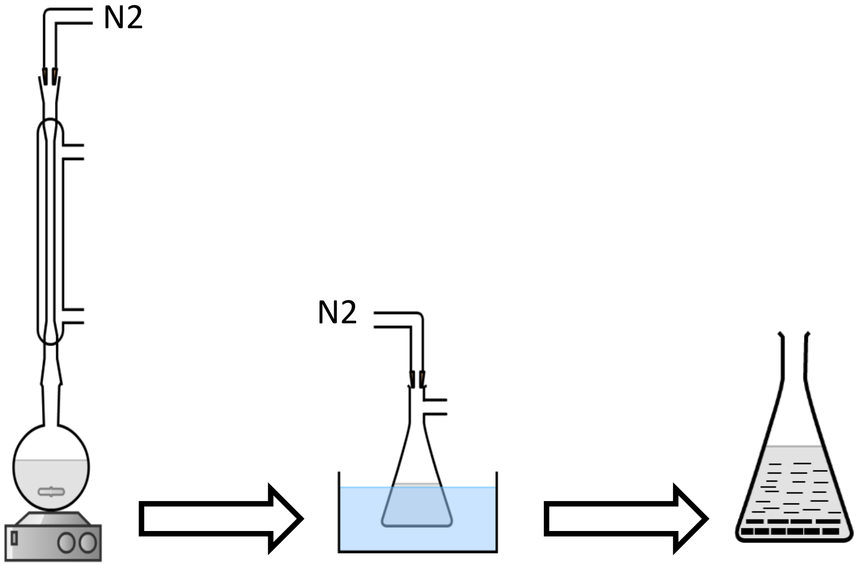
2D Flexible Thermoelectrics

Supervisor: Sir Prof Koysta Novoselov

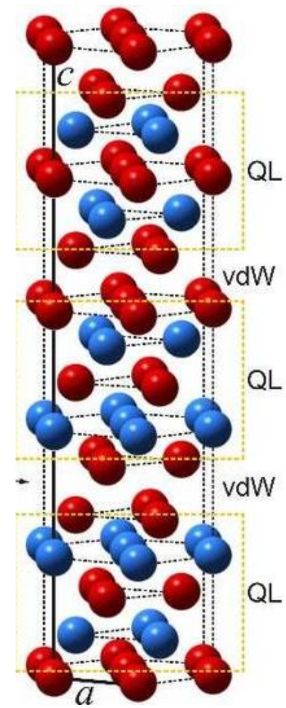
Results are confidential due to the nature of the project

Materials/Synthesis

- Bismuth telluride based alloys
- Intercalation-assisted liquid phase exfoliation

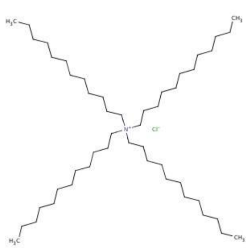


Intercalation Exfoliation Suspension

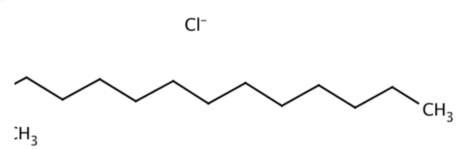


Intercalants:

(2)

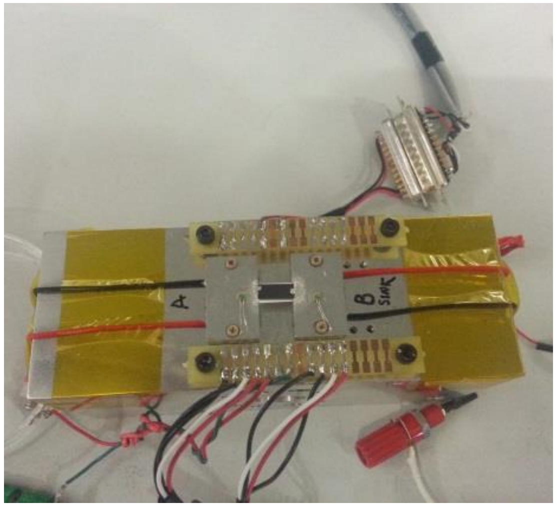


(1)

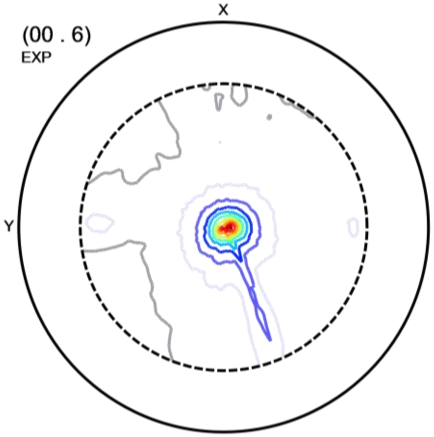


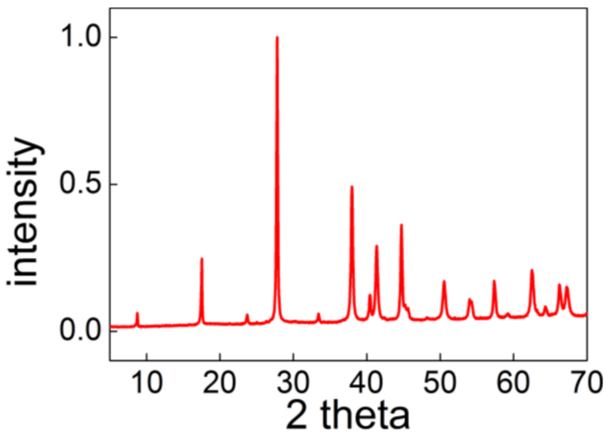
Film Characterisation

- Electrical properties

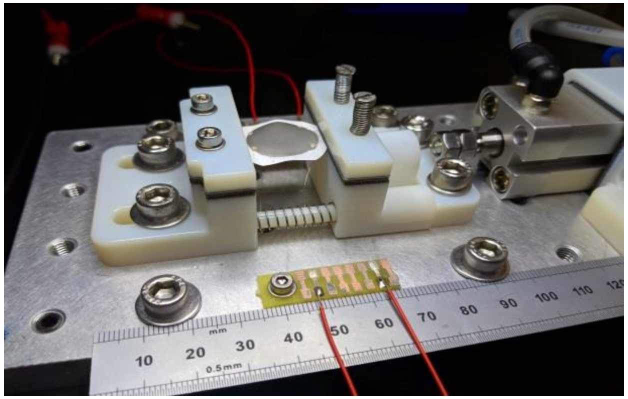


- X-ray Diffraction

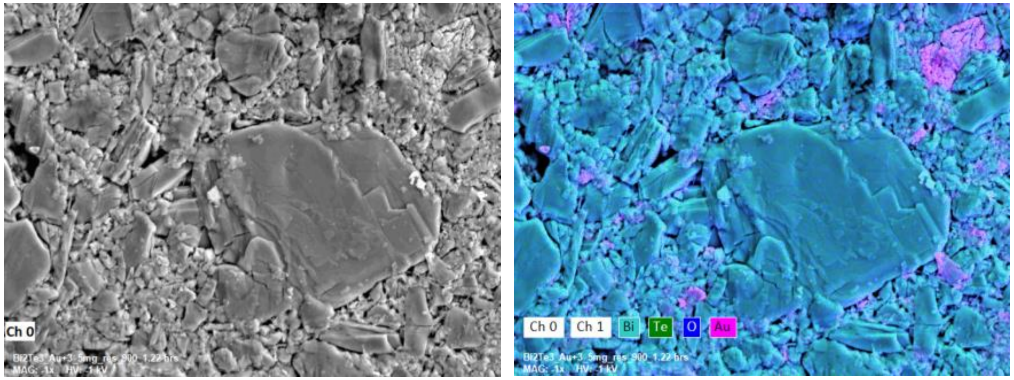




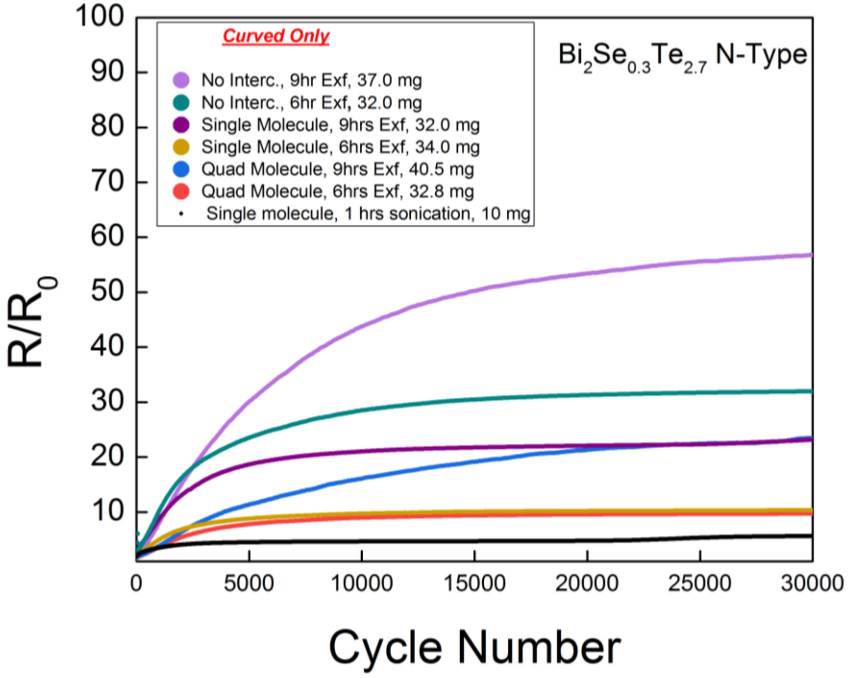
- Durability

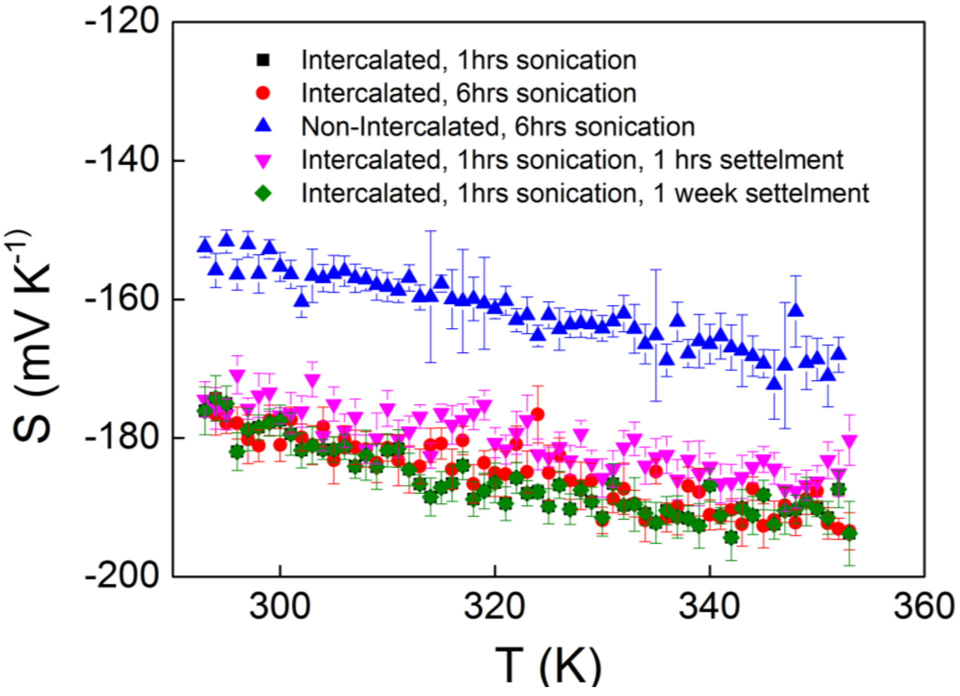


- SEM-EDX / FIB



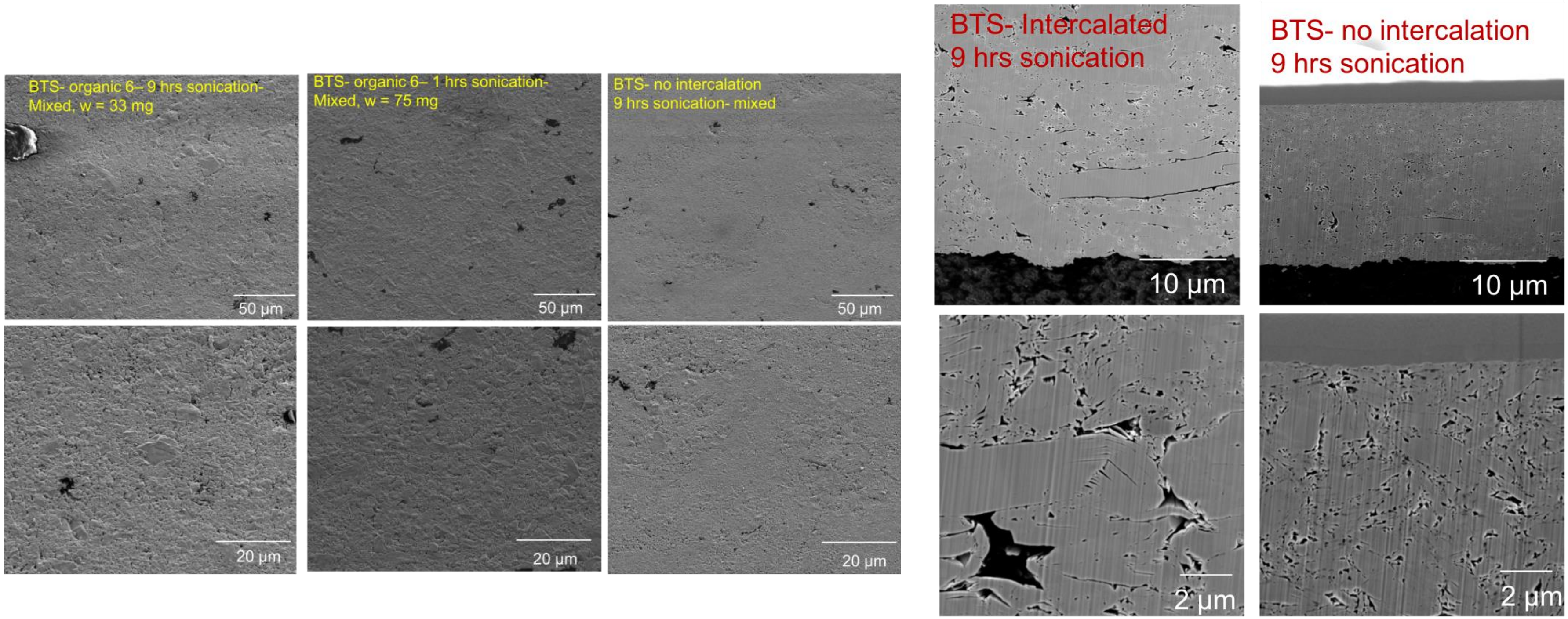
Durability and Electrical Properties





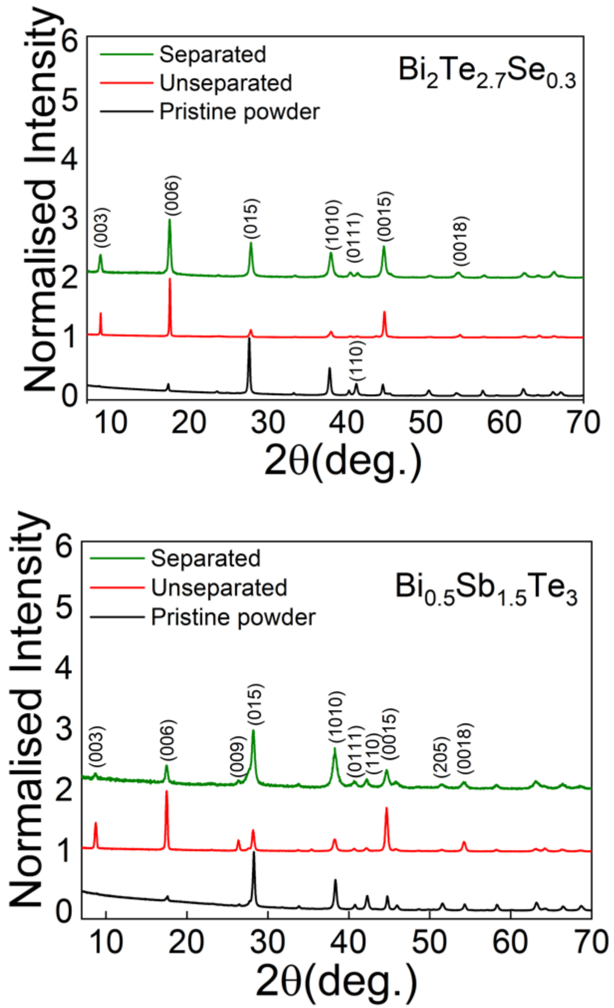
Excelent durability up to 30000 cycle

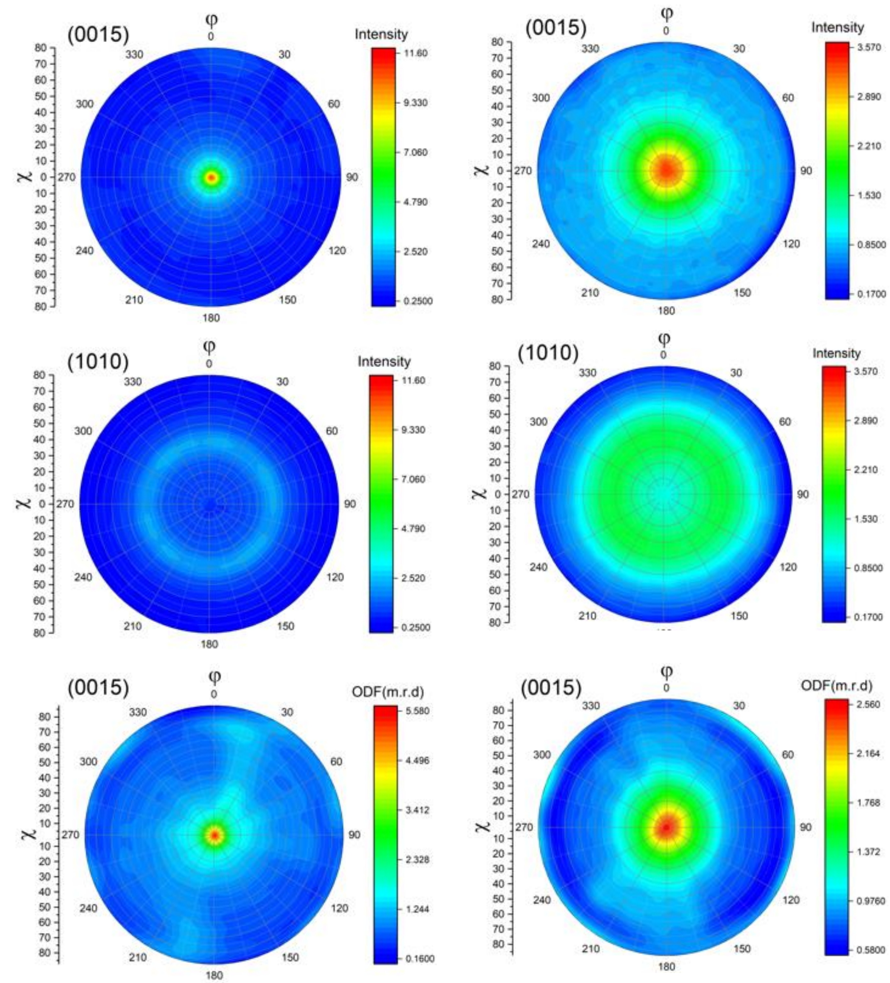
Structural Characterisation



SEM reveals microstructural variations between the intercalated and non-intercalated samples

Structural Characterisation

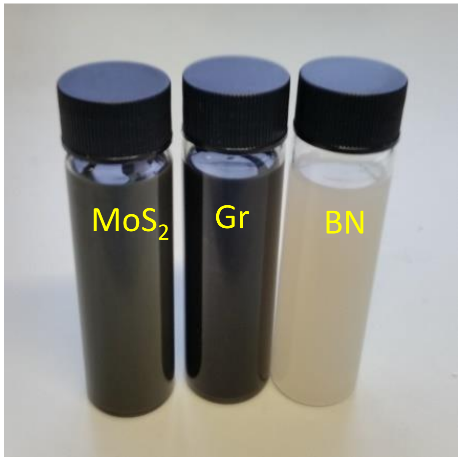


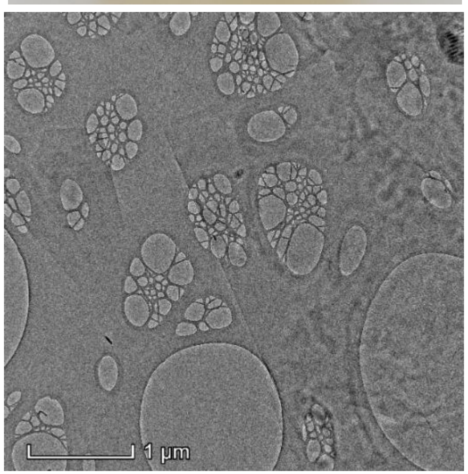


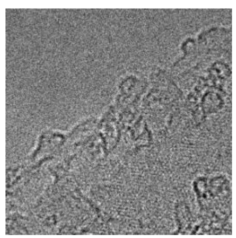
XRD confirms high crystallinity and 00l oriented texture for the prepared films

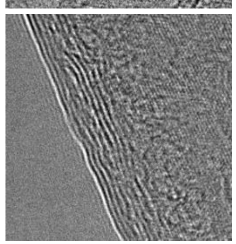
Preferred orientation along c-axis is also confirmed by XRD-pole figures

Additional Projects in the NGI

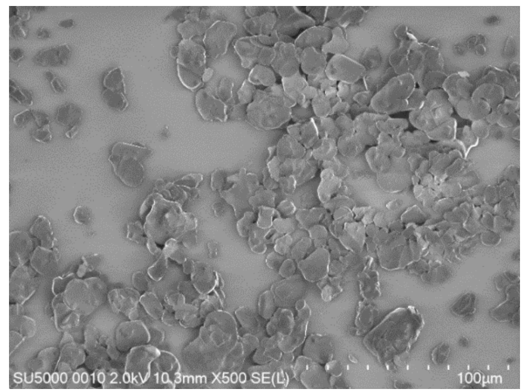


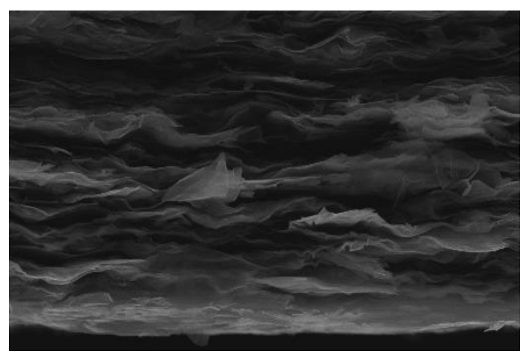


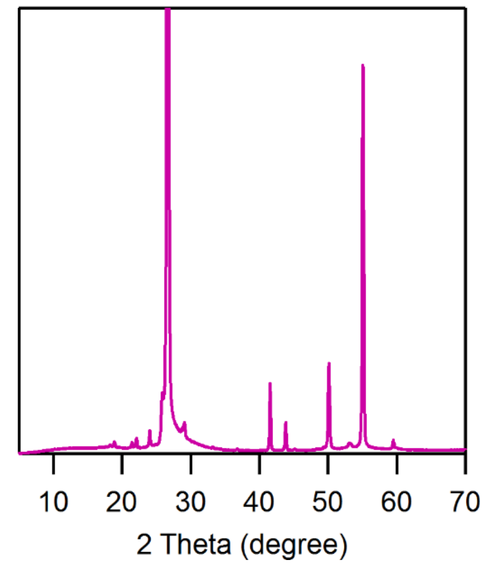




Structural characterisation of Gr, BN, MoS_2







M.Gudarzi, M.Asaad, M.Smith, X.Zhong, R.Gorbachev, K.Novoselov and A.Kretinin,. *npj 2D Mater Appl* **5,** 35 (2021).

Thermoelectric Heat to Electricity Conversion in Molecule-Nanoparticle Networks

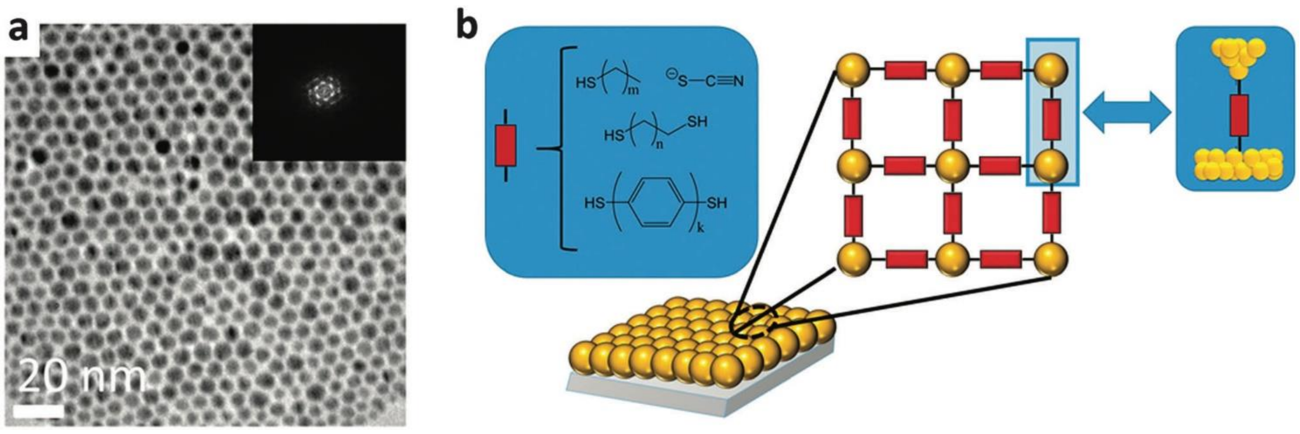
Principle Investigator: Jan Mol

Aim

Molecule-nanoparticle networks: Scalability of molecular junction thermoelectrics

Aims:

- Synthesising ordered arrays of gold nanoparticles cross-linked by molecules:
    - Various organic molecules and chemical routes to be investigated.
- Structural and thermoelectric characterisation of the fabricated devices.

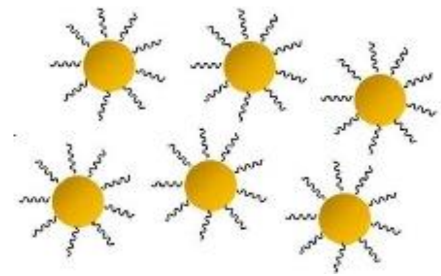


W. B. Chang et al. *Phys.Chem.Chem.Phys.,* 2015, 17, 6207

Synthesis

Step one: Synthesis of hydrophobic AuNPs:

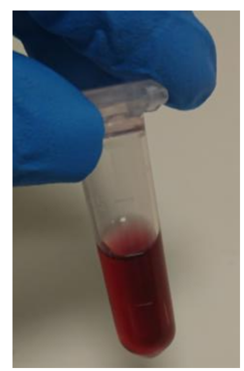
$HAuCl_4$ + Oleyelamine (OAm) $\xrightarrow[\text{200 Cdeg}]{\text{Toluene,}}$



Dark red colour

(surface plasmon resonance)

Wash with MeOH $\longrightarrow$ Re-disperse in Hexane

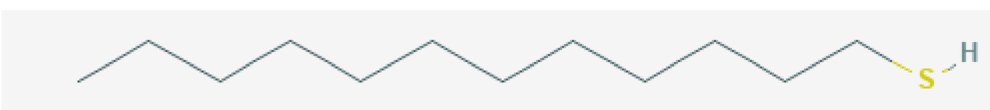


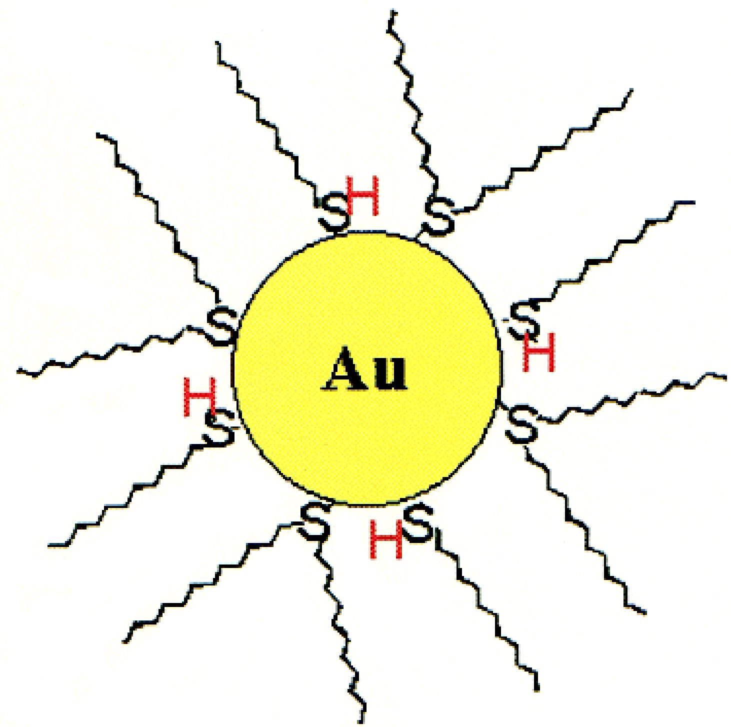
Synthesis

Step 2: Ligand exchange: Alkanethiols

$$\text{Au-OAm} \xrightarrow[\text{Left overnight to precipitate}]{\text{Excess Dodecanethiol}} \text{black waxy precipitate}$$

1-Dodecanethiol



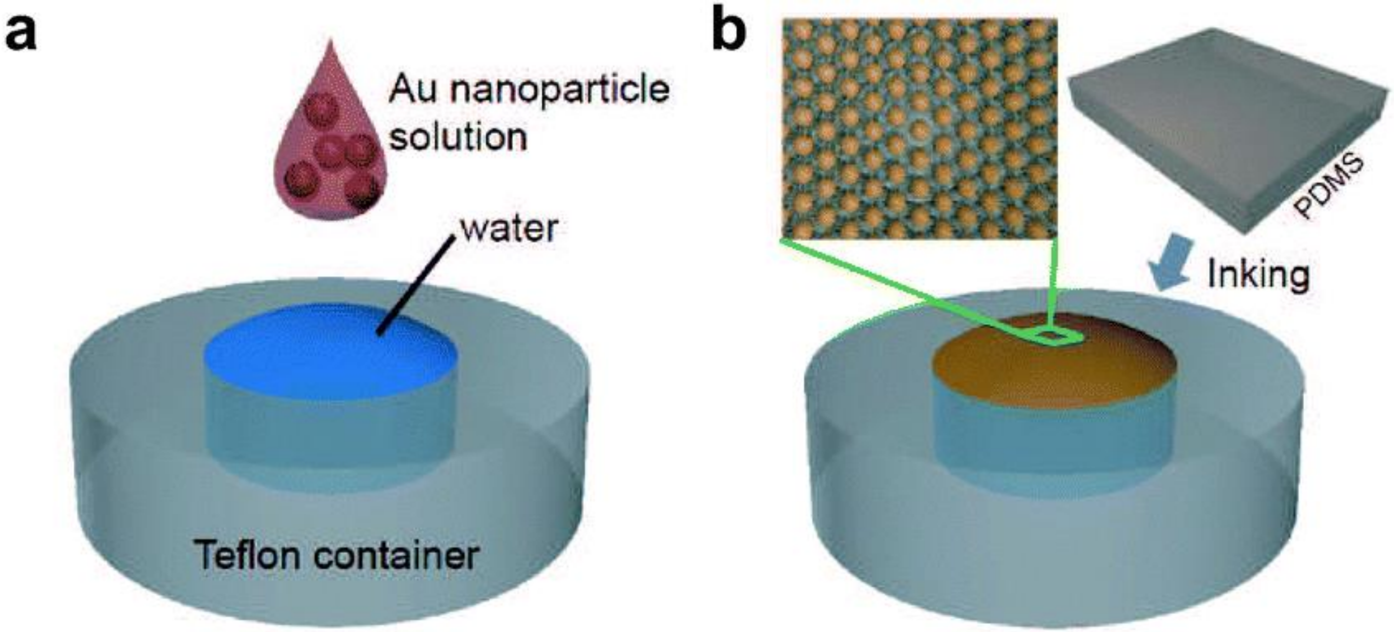


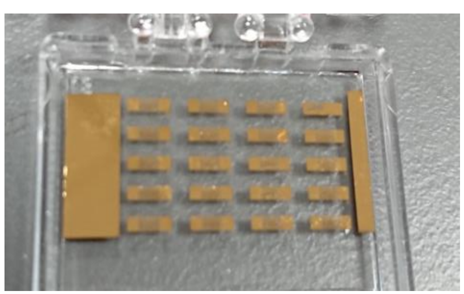
Dodecanethiol:

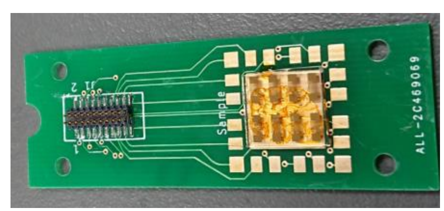
They serve as stabilizing agents to prevent nanoparticles from aggregating they act as tunnel barriers in charge transport through the final arrays structure

Device fabrication and characterisation

Drying-mediated assembly on water surface

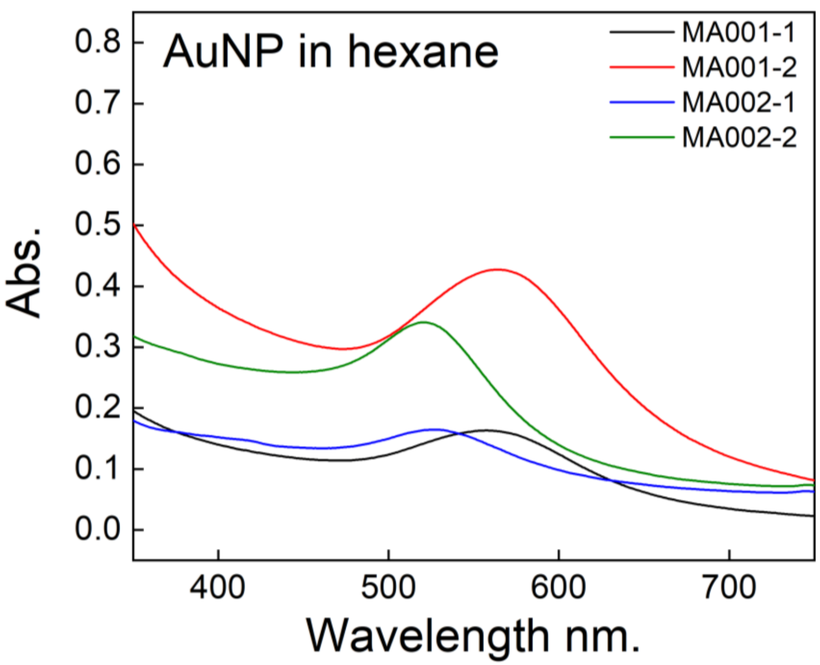




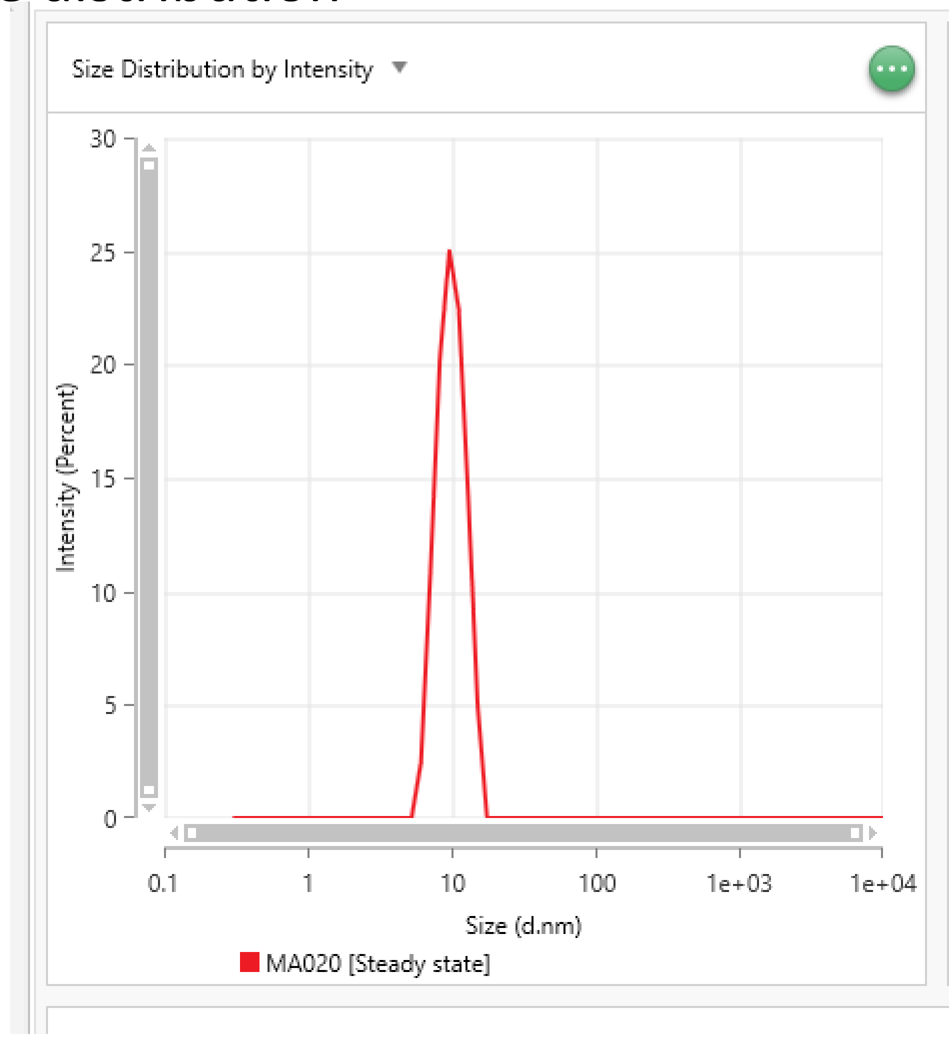


Characterisation

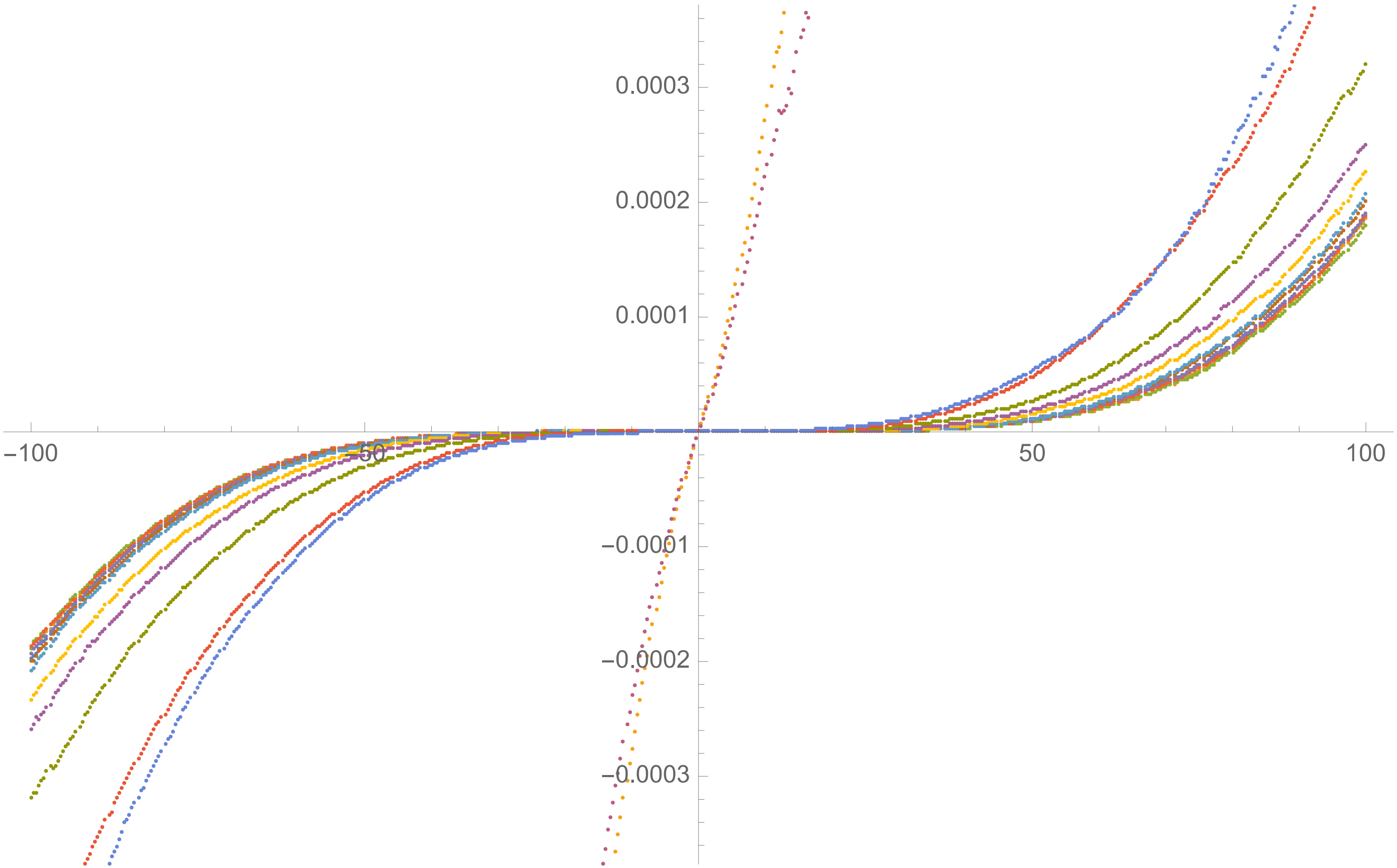
UV-Vis : size



Dynamic light scattering using Zetaziser: size distribution



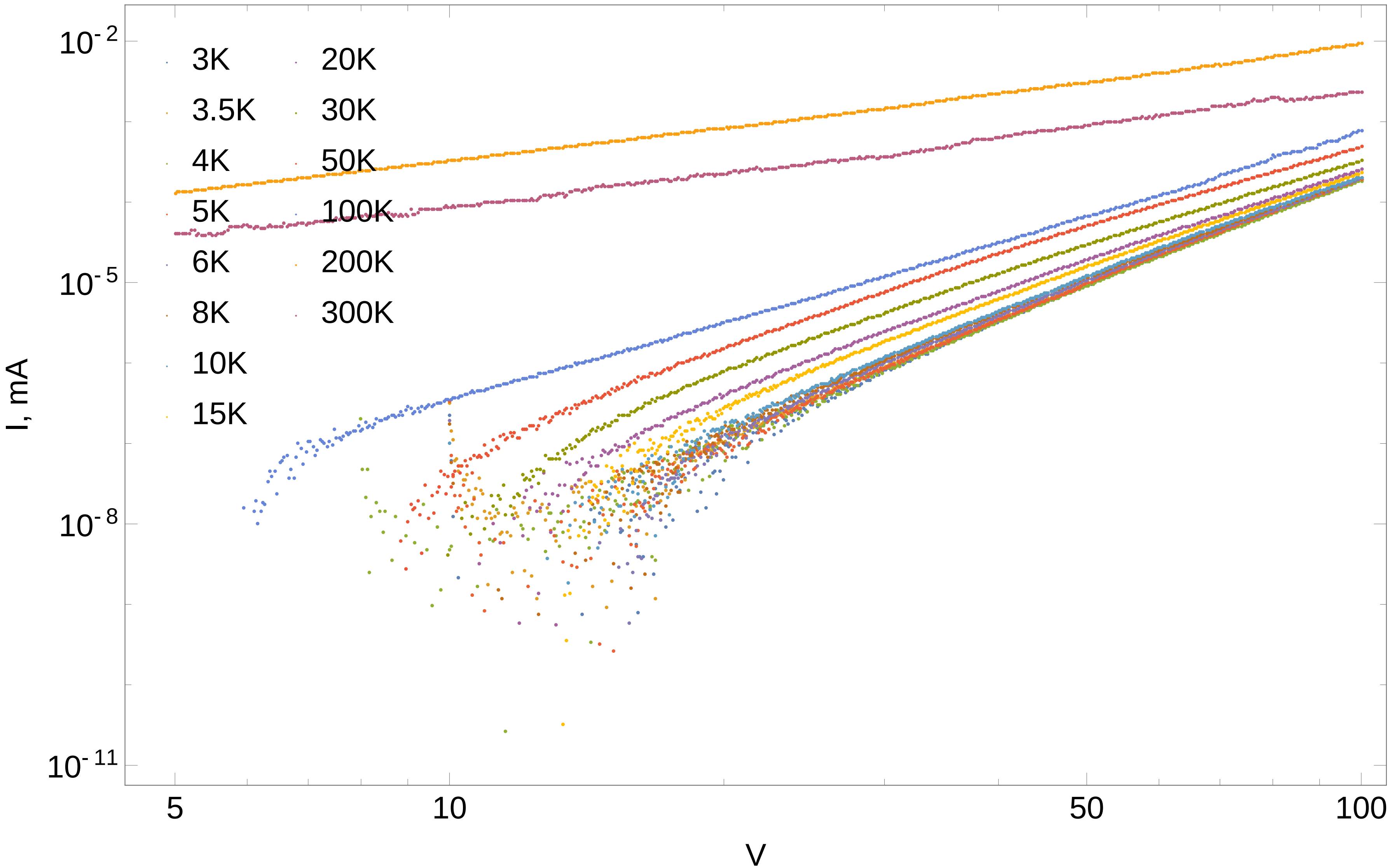
Electrical characterisation, Dodecanethiol $C_{12}SH$



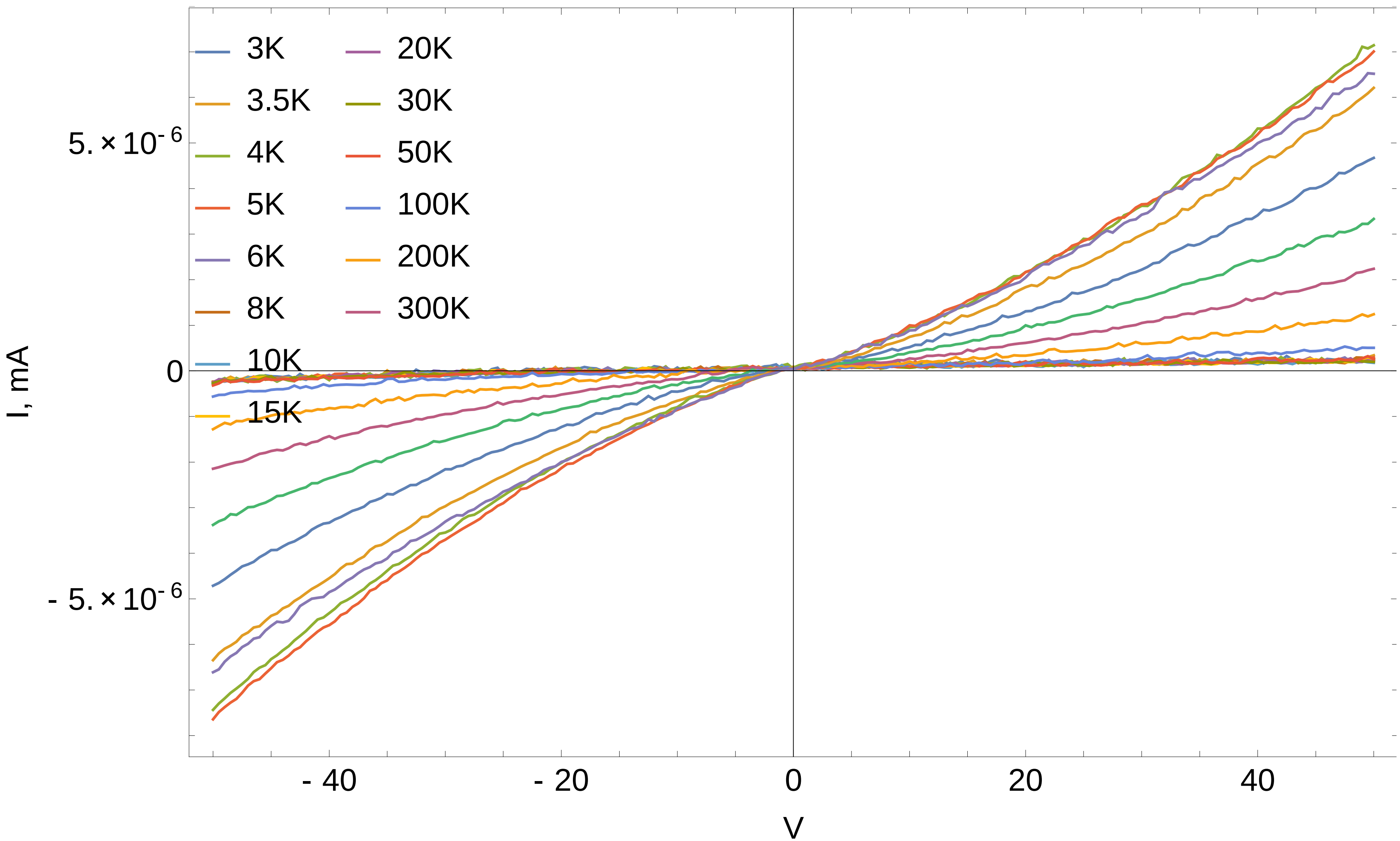
Results are consistent with literature

Electrical characterisation, Dodecanethiol $C_{12}SH$

IV traces on log-log scale

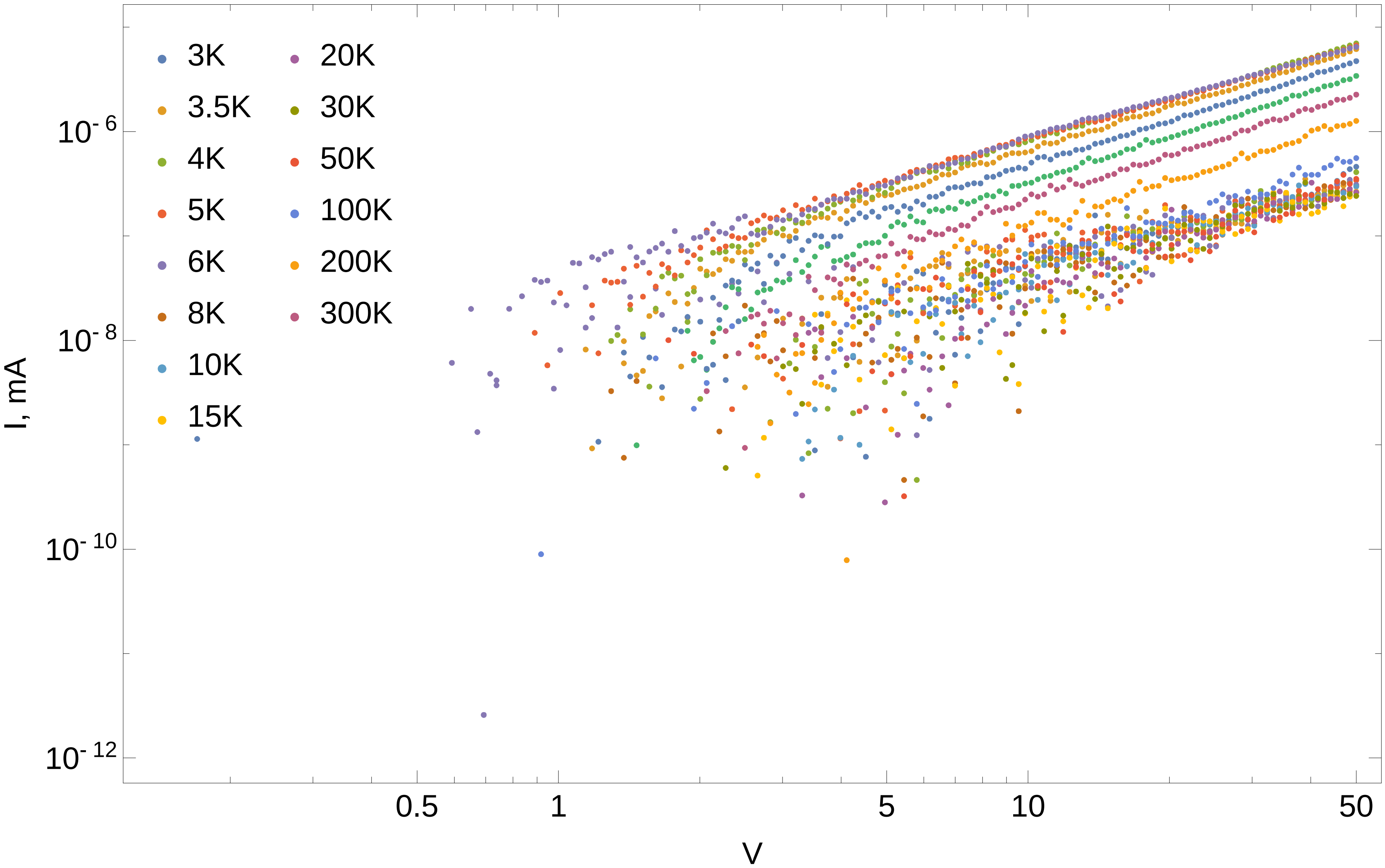


Electrical characterisation, Ocanethiol C_8SH

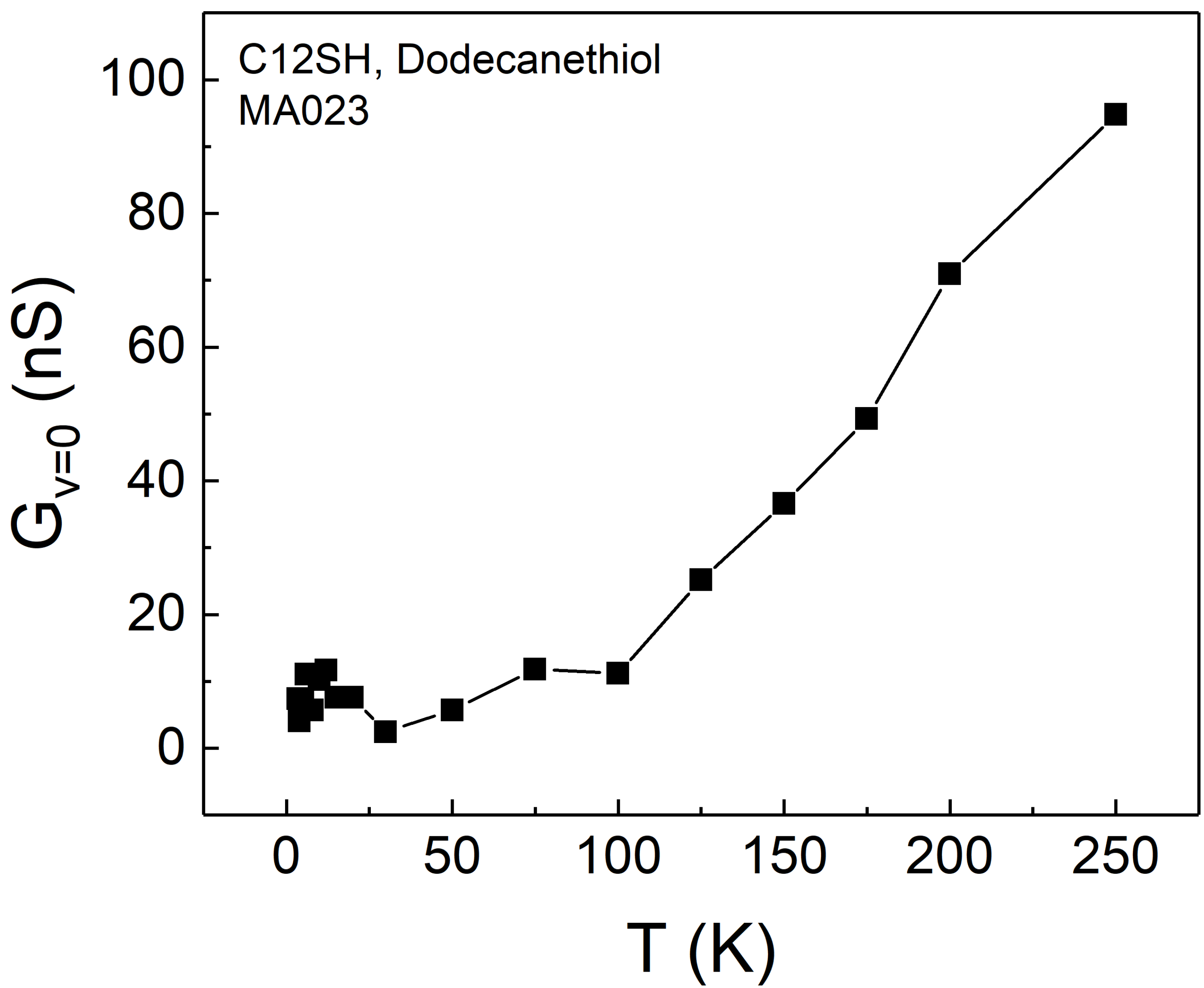


Electrical characterisation, Ocanethiol C_8SH

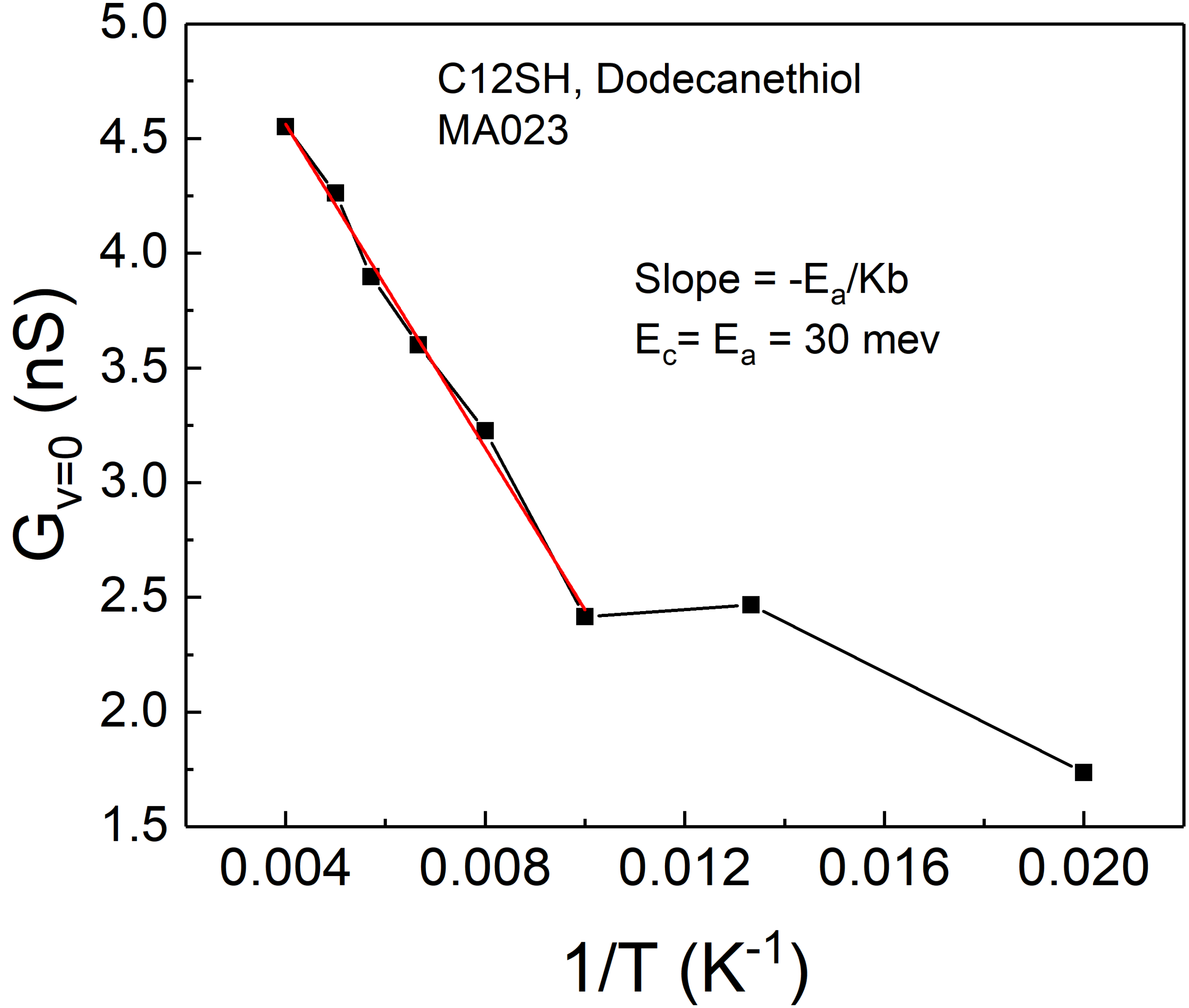
IV traces on log-log scale



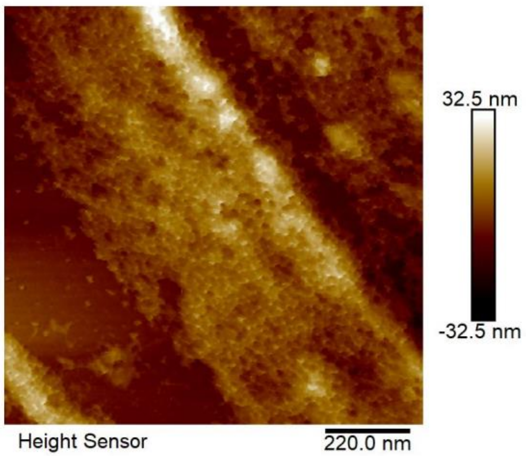
Conductance

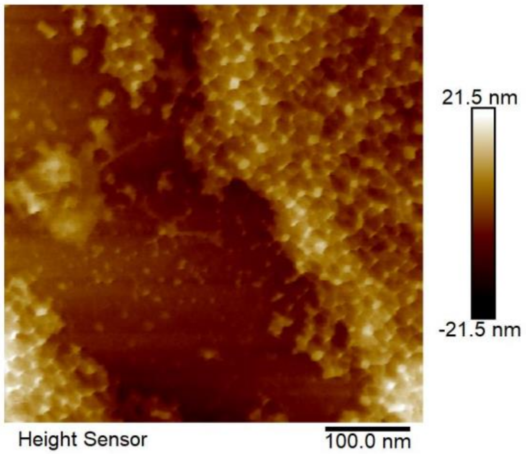


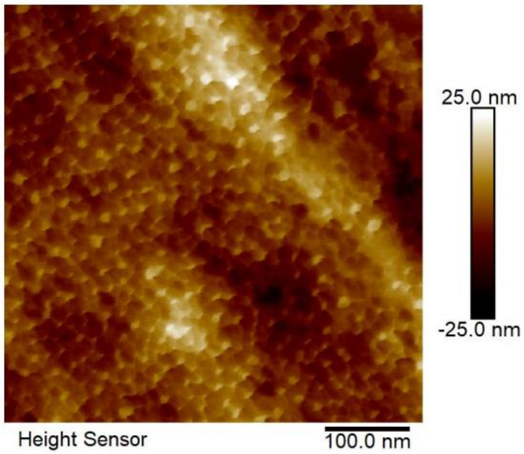
Activation Energy

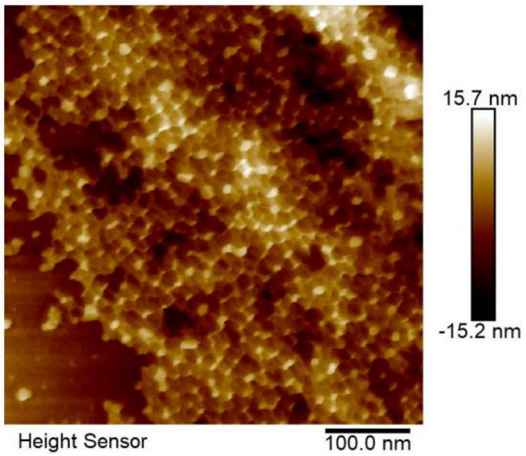


Structural Characterisation, Octanethiol C_8SH









Conclusions

- My PhD research focused on half Hesuler thermoelectrics , and the obtained results provide novel and important contribution to the literature

- During my first postdoc at the NGI, I developed flexible,
high efficient thermoelectric films based on Bismuth Telluride and Antimony Telluride alloys

- My project in Queen Mary is focused on fabricating devices based on AuNPA
- crosslinked by molecules for TE heat to electricity conversion:
- Investigation different molecules
- Measuring Seebeck coefficient and thermal conductivity of the arrays and eventually
- calculating ZT
- Structural characterization of the fabricated arrays

Thank you for listening!