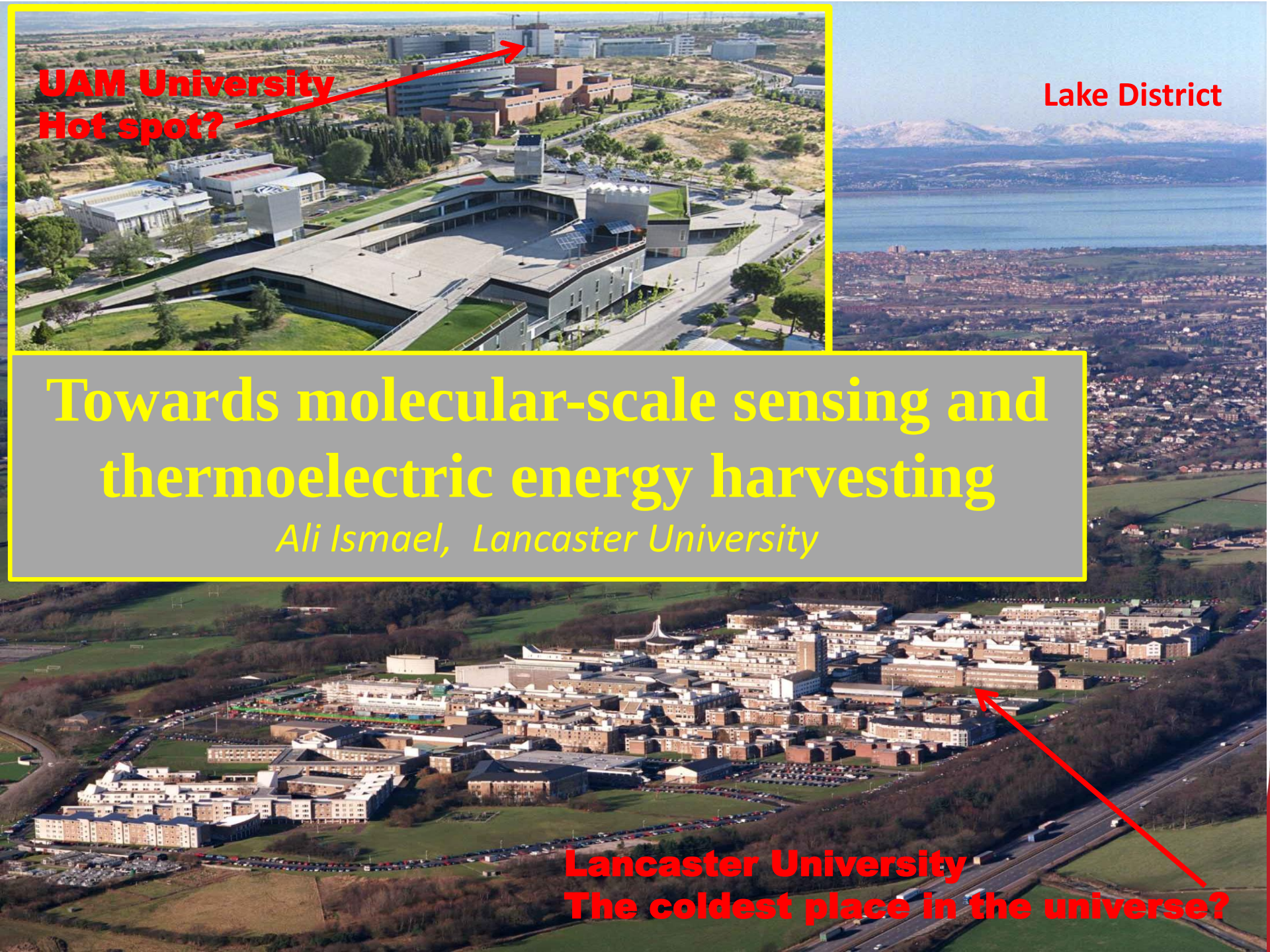
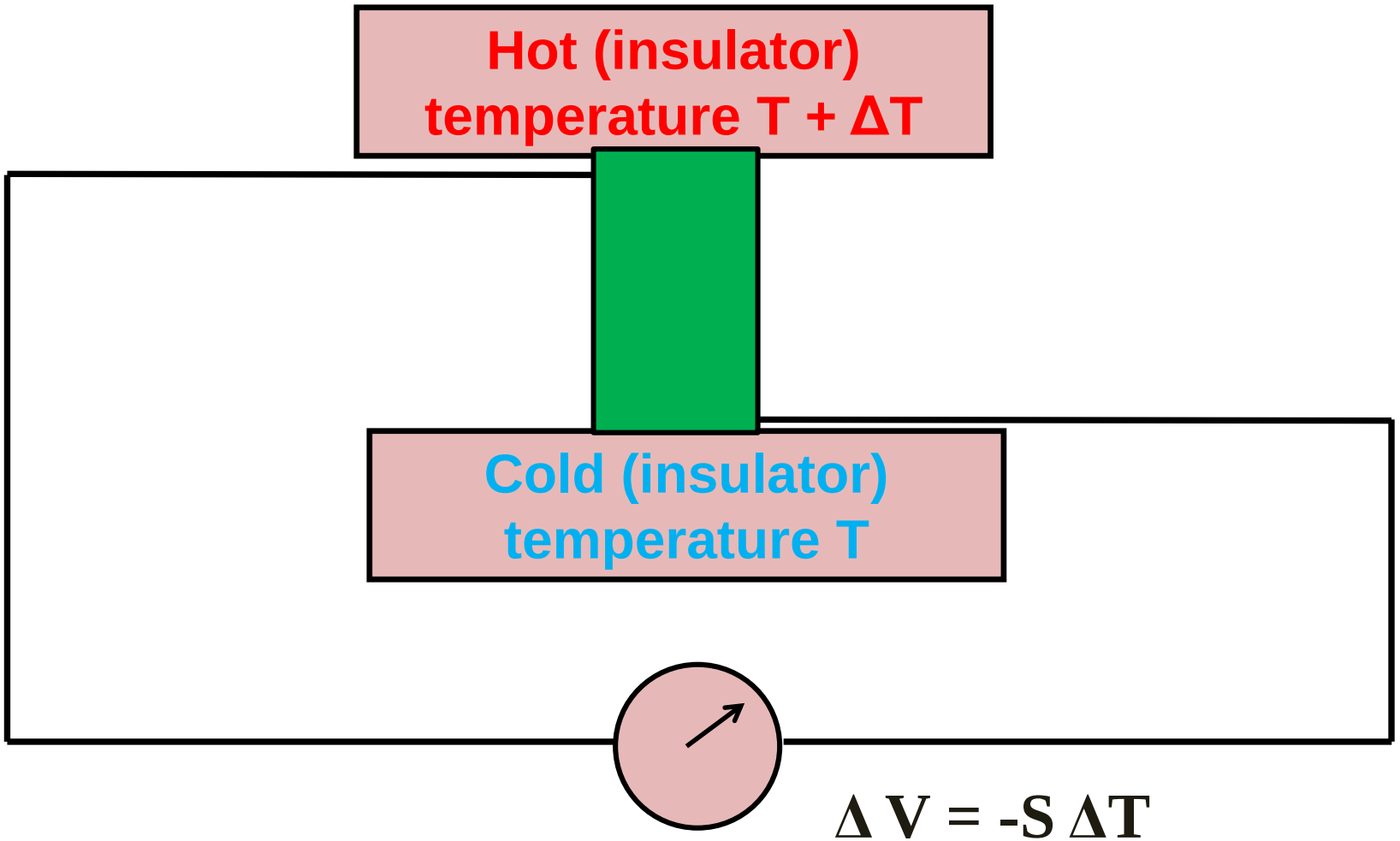

UAM University
Hot spot?
Lake District
Towards molecular-scale sensing and thermoelectric energy harvesting
Ali Ismael, Lancaster University
Lancaster University
The coldest place in the universe?

Outline

Introduction to thermopower

- **Three examples of my PhD projects:**
  - **Sensing by crown-ether-bridged anthraquinones**
  - **Thermoelectric properties of crown-ether-bridged anthraquinones**
  - **Thermoelectric properties of fullerenes and endohedral metallofullerenes**

Definition of thermopower (S)



AIP The Journal of Chemical Physics

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Full . Published Online: February 2017 Accepted: January 2017

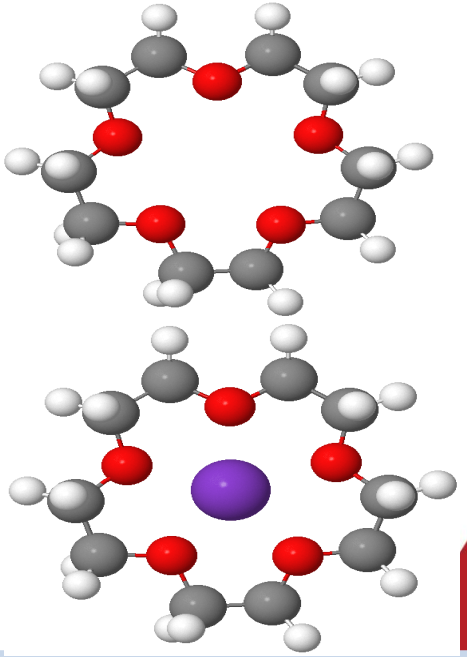
Discriminating single-molecule sensing by crown-ether-based molecular junctions

The Journal of Chemical Physics **146**, 064704 (2017); https://doi.org/10.1063/1.4975771

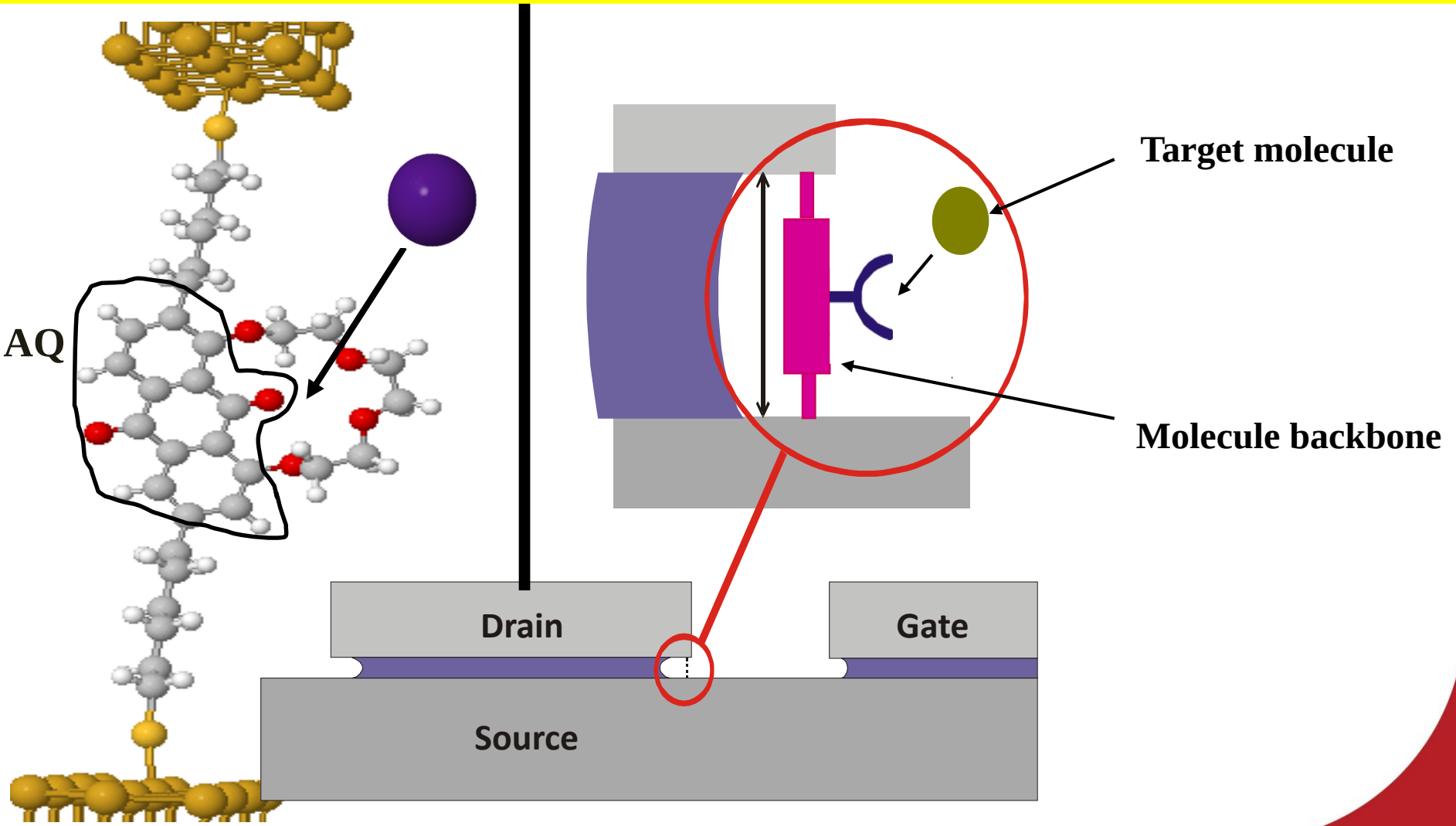
Ali K. Ismael[1,2], Alaa Al-Jobory[1,3], Iain Grace[1], *and* Colin J. Lambert[1]

Why crown ethers?

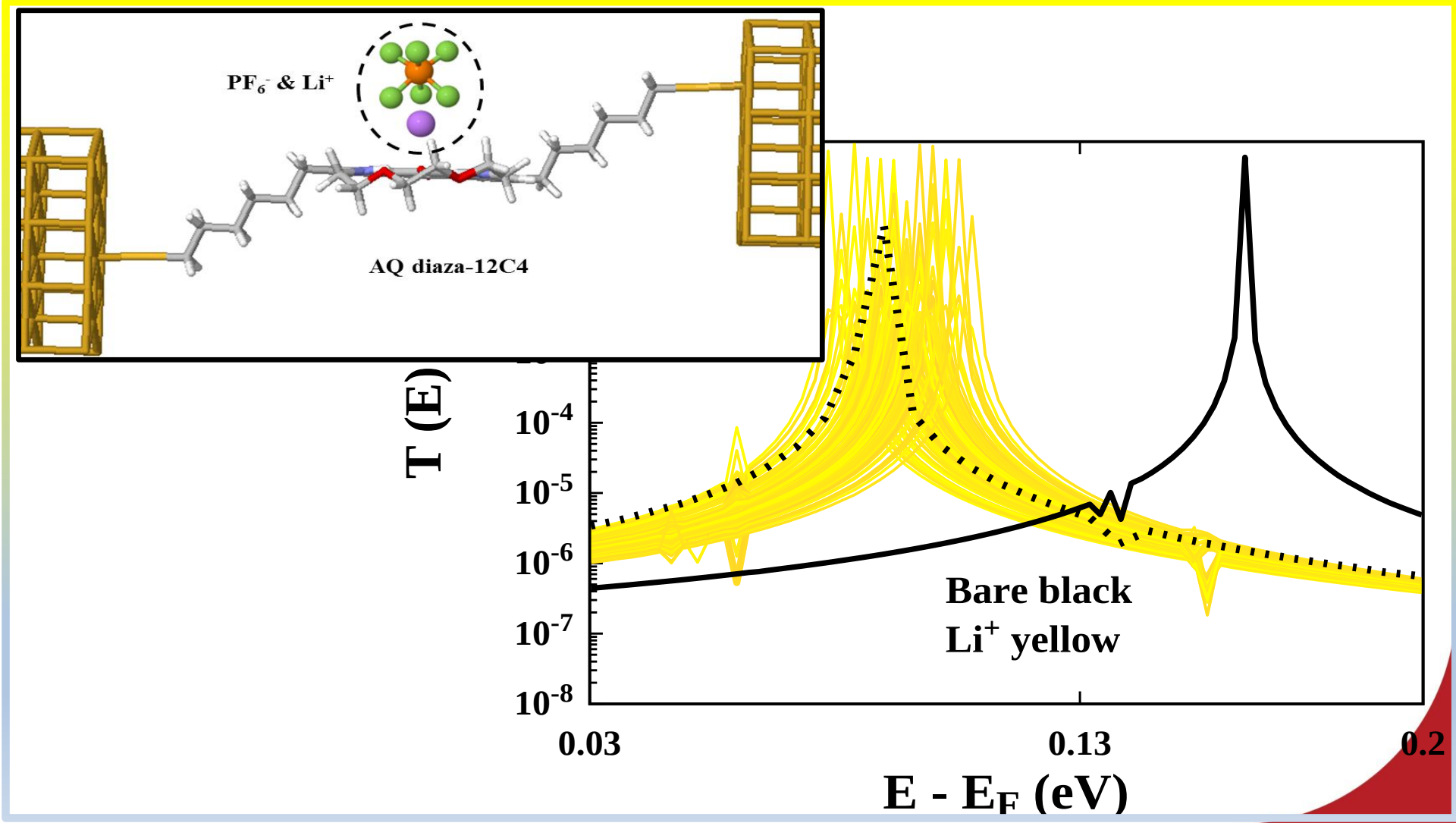
- Crown ethers are well-known to selectively bind ions
- Chemical sensor (Sensing of alkali metals)
- Applications: switches, memory devices, transistors, rectifiers.
- Medical and biomedical applications, removal of harmful metal ions or supply of essential metal ions and in cancer treatment



A molecular sensor



Sensing a Li+ Counter ion



Effect of different cavity size and captured cation on T(E)

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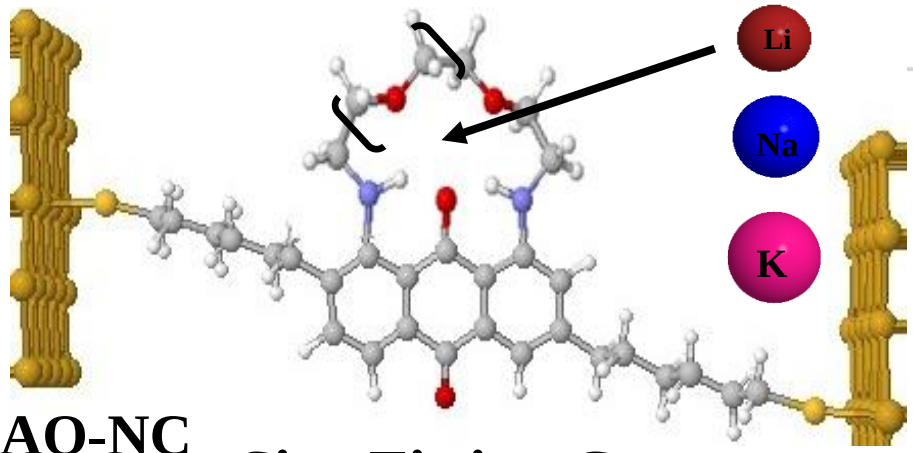
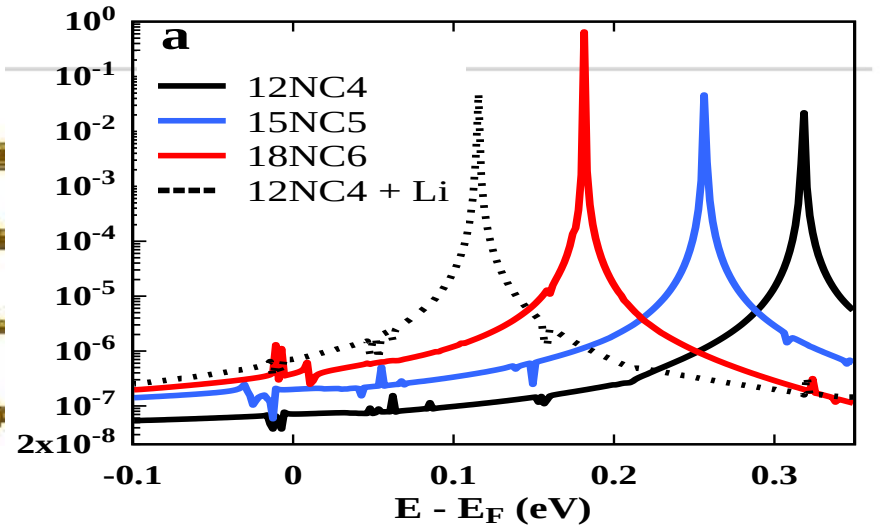
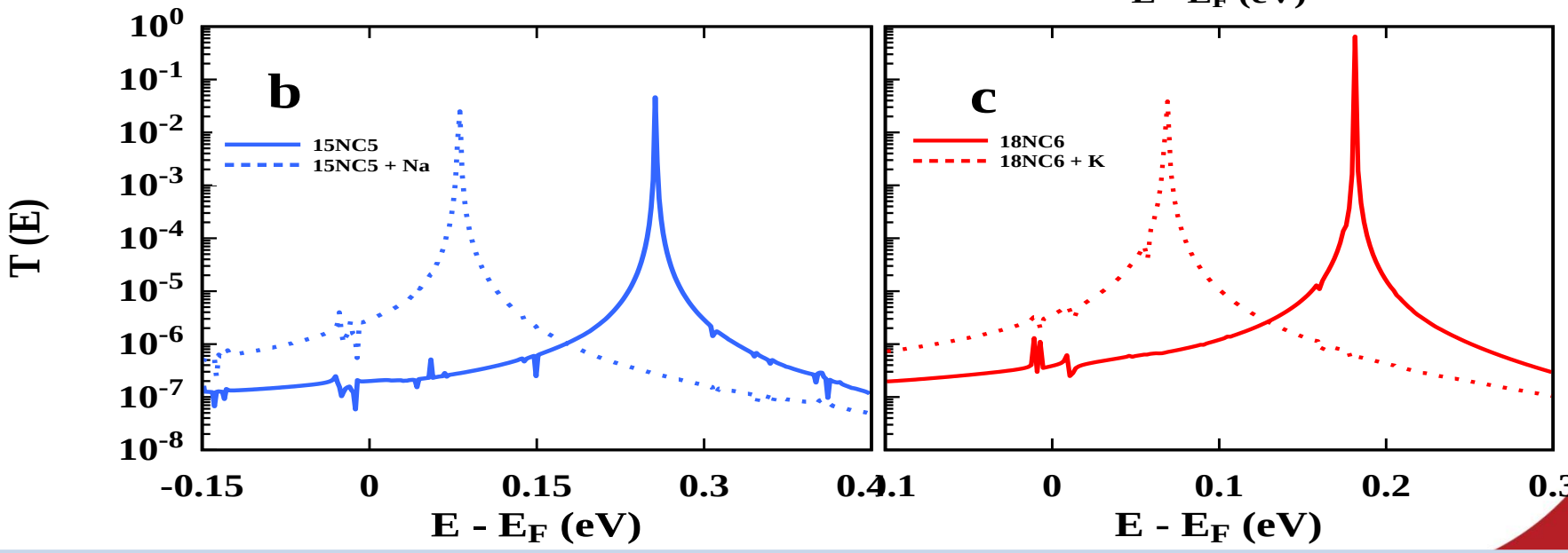


AQ-NC

Size-Fitting Concept





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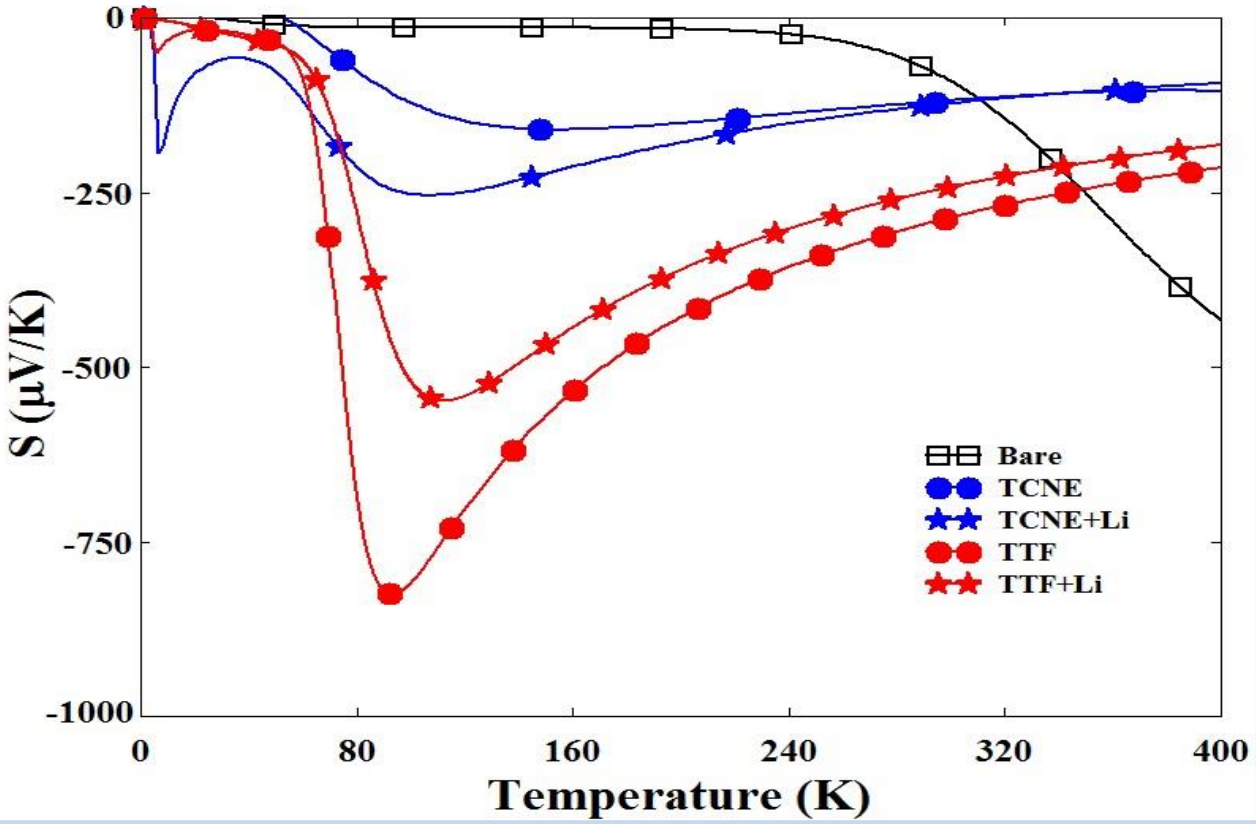
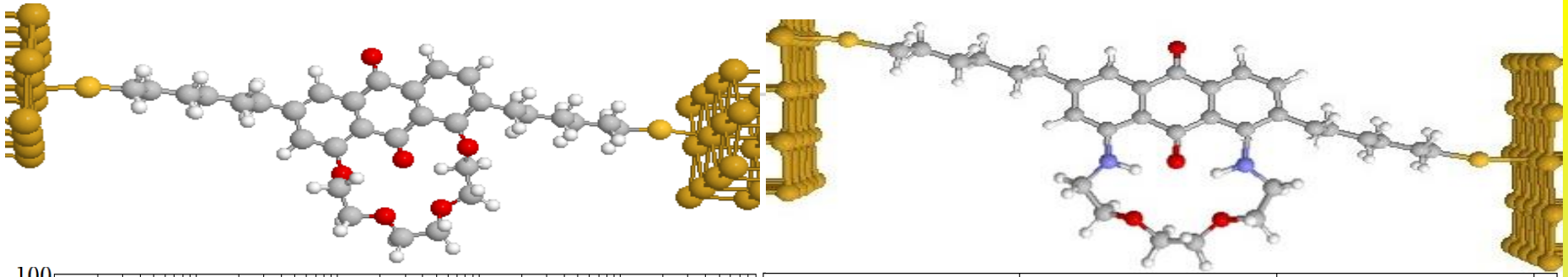
Increasing the thermopower of crown-ether-bridged anthraquinones†

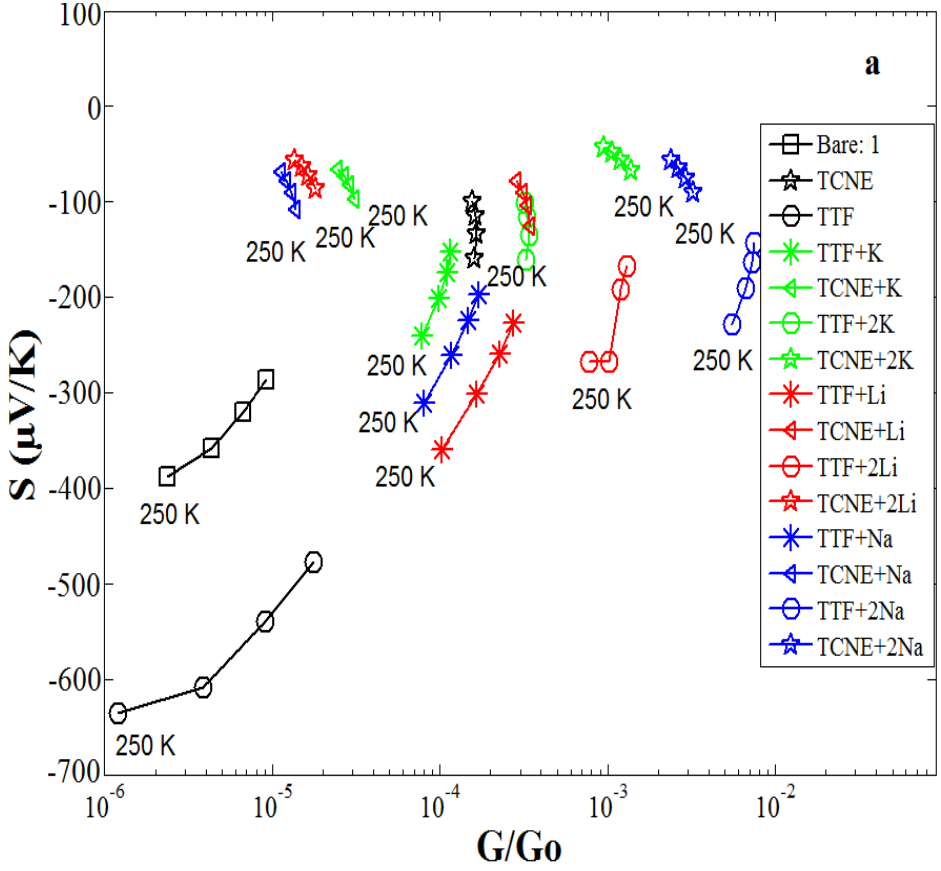
Ali K. Ismael,[a,b] Iain Grace[a] and Colin J. Lambert*[a]

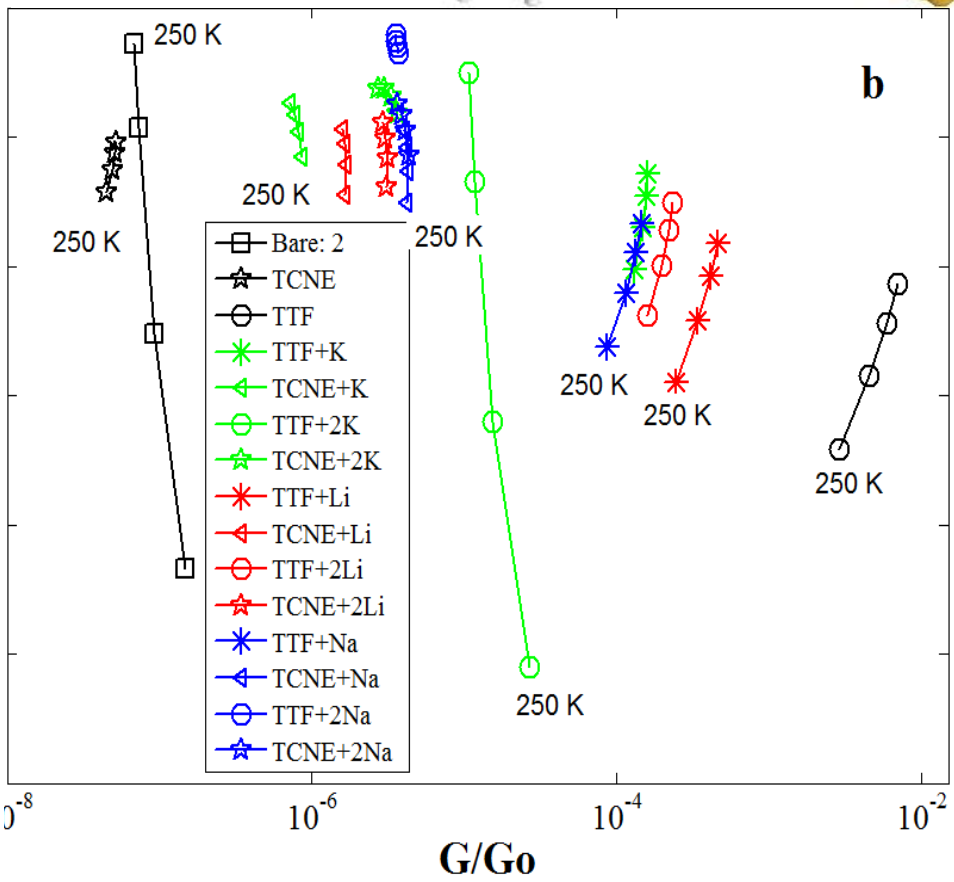
Does the sensing feature enhance S? Thermopower of complexes



S – G Map of AQ-OC & AQ-NC







Conclusions

- Crown ethers selectively bind individual ions
- Conductance increase depends on the ion and the size of the ligand
- Opens up possibility of sensing individual ions through careful design of the crown moiety.
- Complex formation produces significant gains in the thermopower up to $\boldsymbol{S \approx -600}$ **&** $\boldsymbol{S \approx -400\ \mu V/K}$ **at room temperature**

nature materials

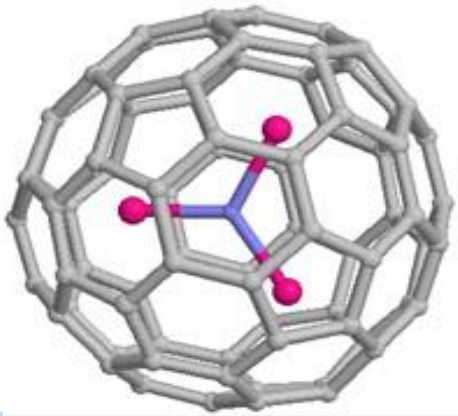
LETTERS

PUBLISHED ONLINE: 7 DECEMBER 2015 | DOI: 10.1038/NMAT4487

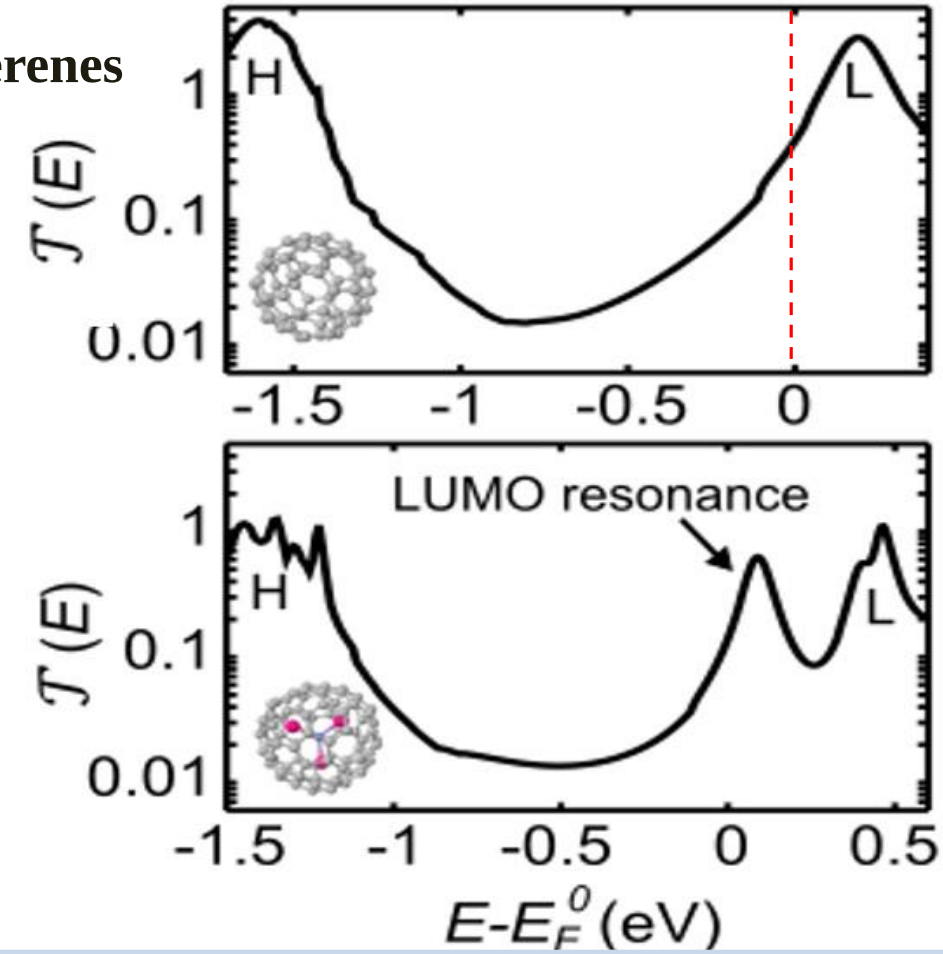
Molecular design and control of fullerene-based bi-thermoelectric materials

Laura Rincón-García[1,2], Ali K. Ismael[3,4], Charalambos Evangeli[1], Iain Grace[3], Gabino Rubio-Bollinger[1,5], Kyriakos Porfyrakis[6], Nicolás Agraït[1,2,5]* and Colin J. Lambert[3]*

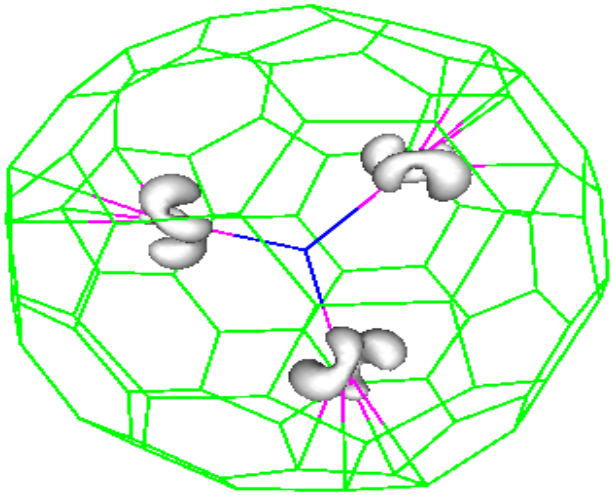
Fullerenes and Endohedral Metallofullerenes



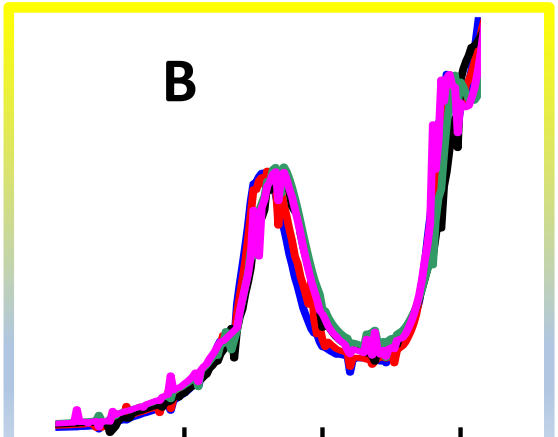
- Do fullerenes accommodate atoms inside their cages?
- What is the effect of the metallic part on the T(E) and S?

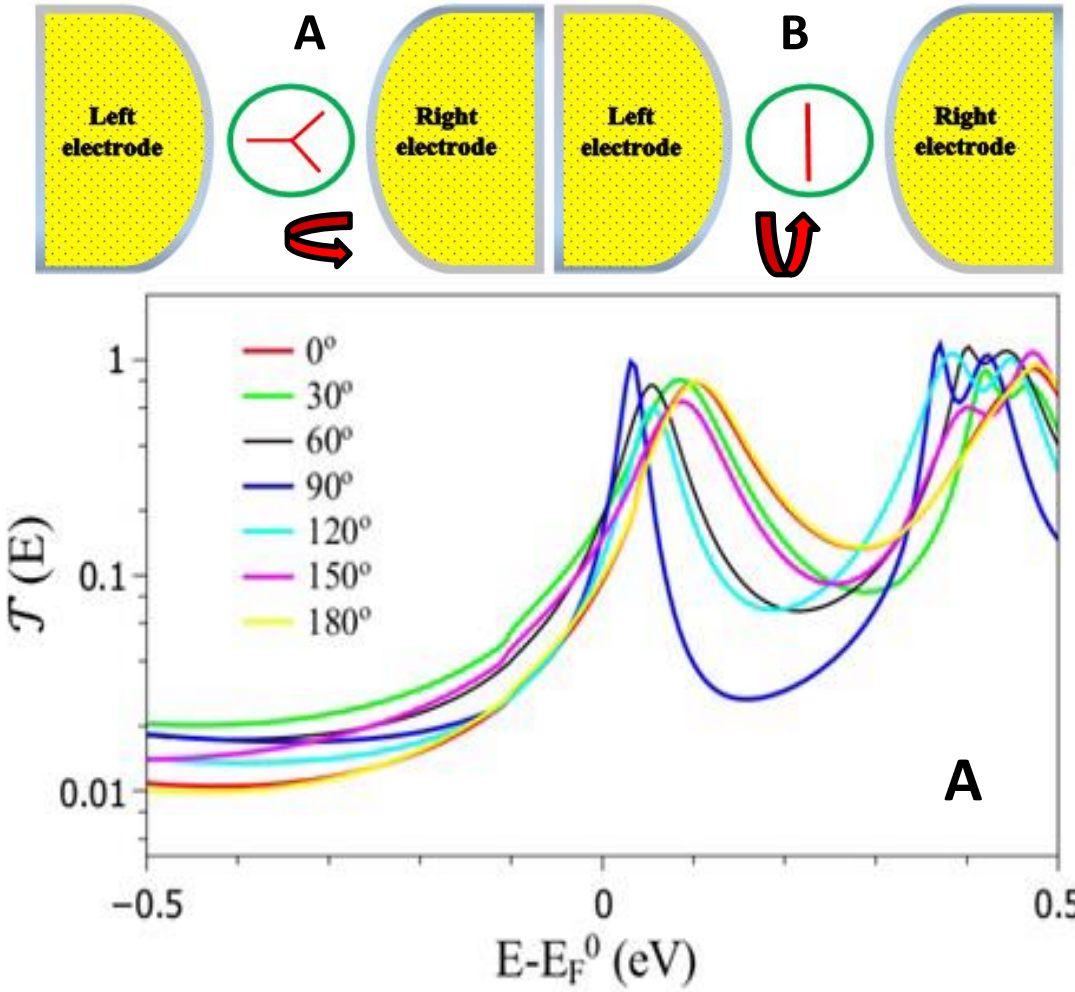


Is the LUMO resonance due to the metallic part (Sc_3N)?

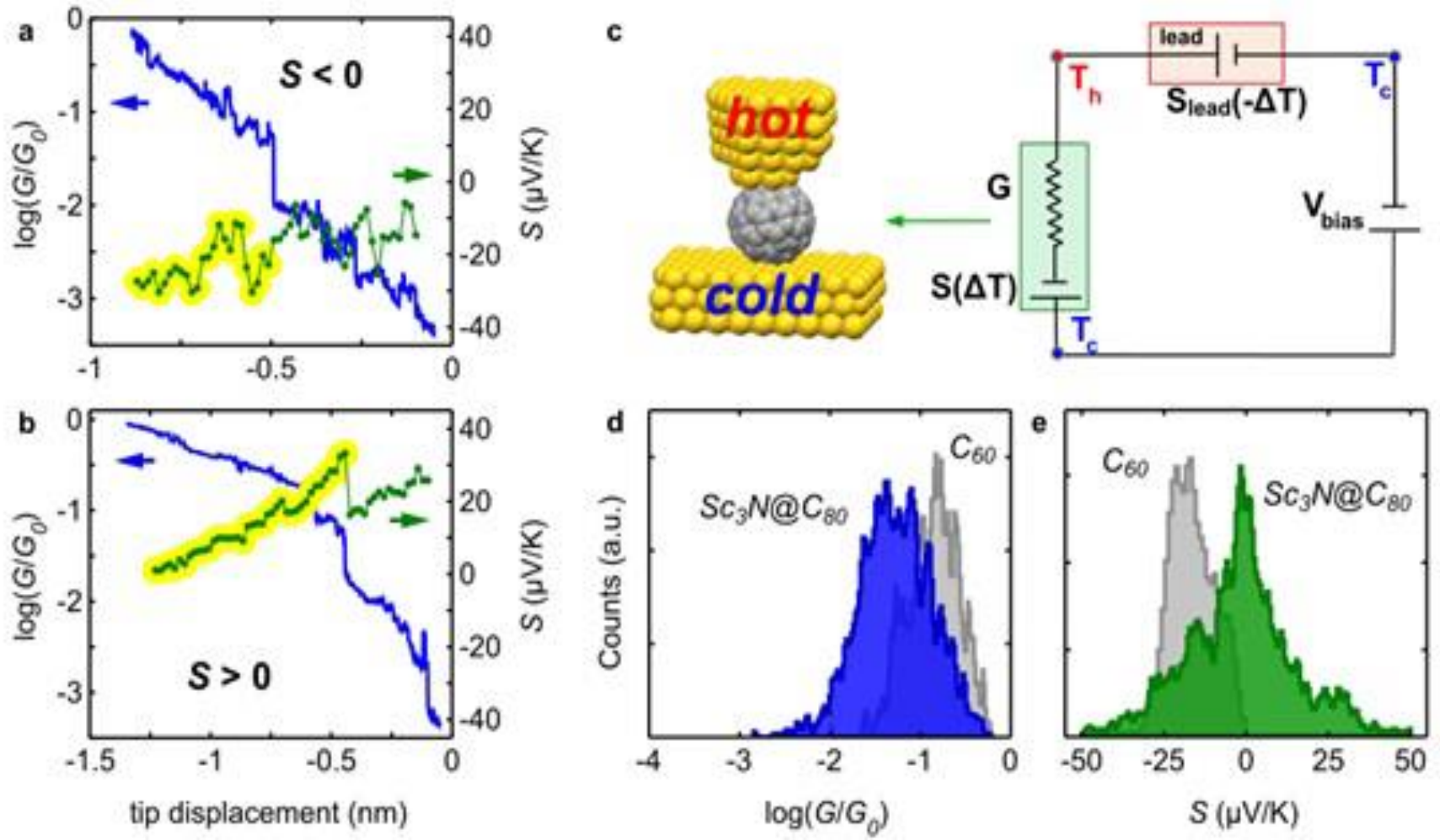


LDS $Sc_3N@C_{80}$





Experimental Measurements C_{60} & $Sc_3N@C_{80}$



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Both theory and experiment

- Extra resonance due to the metallic part (**Sc_3N**) inside the cage
- Conductance for **C_{60}** is higher than **$Sc_3N@C_{80}$**
- Thermopower of **C_{60}** always negative, whereas for **$Sc_3N@C_{80}$** negative or positive (Bi-thermal)

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Thank you for listening!

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