DTC Studentship Proposal

PROJECT DETAILS

Title: Conductive Polymers and Polymer Nanocomposites for Flexible Thermoelectrics - "NANOFLEXTE".

Principal Investigator: Emiliano Bilotti (EB).

MOTIVATION FOR THE PROJECT

Concept and objective:

The ultimate objective is to develop a novel textile, based on organic thermoelectric materials, for utilisation in electrical to thermal energy conversion and vice-versa and that can also be manufactured in large scale. These will then have wide-ranging potential applications, such as personal climate control in garments, wearable micro-generators for bio-sensors and devices, and as large scale fabric parasols for solar power generation in buildings. With an advantaged performance/cost structure, this will lead to substantial economic and environmental benefits, and will also utilise abundant materials in order to deliver an overall lower transaction cost than existing materials. Increasing scale-up in production will have further positive effects on cost reductions.

Scientific challenge: For practical applications it is important to improve the efficiency of current TE devices. The TE efficiency is determined by the dimensionless TE figure of merit, $zT=S^2\sigma T/k$, where S is Seebeck coefficient, σ is electrical conductivity and k is thermal conductivity. The zT of the most widely used TE materials (alloys like Bi_2Te_3 and Sb_2Te_3), reaches values of about 1 [1]. No commercial TE products are currently based on organic materials [2]. This is due to the fact that polymers generally present very low electrical conductivity. Nevertheless the use of conjugated polymers (particularly semiconductors), and the incorporation of (semi-)conductive (nano-)particles into a polymeric matrix, promise to offer an interesting alternative to inorganic TE. This is due to the the possibility of decoupling electrical conductivity from thermal conductivity, together with low weight, lower costs and easy processability. Using materials at the nano-scale (nanofillers) will allow to further reduce the thermal conductivity by an increased phonon scattering without affecting the electrical conductivity, as demonstrated for bulk silicon and Si nanowires [3]. Recently Bubnova *et al.* [4] presented the highest value of zT yet achieved for conductive polymers. By controlling its oxidation level the power factor ($S^2\sigma$) of a conducting polymer PEDOT-Tos could be optimised (6-fold increase) and the zT reached 0.25 at room temperature. Previously Kim et al. [5] studied the effect of a number of parameters (e.g. CNT type and concentration, polymer matrix, processing conditions) on the thermoelectric properties of a series of CNT-polymer composites. The presence of CNT improved the zT of the virgin polymer to 0.02.

Originality: It is believed that a systematic approach into the selection of the most appropriate conductive polymers and/or types and loadings of conductive nanofillers (with high thermopower and electrical conductivity), and control of the structure, morphology and doping level can result into significant improvement in the efficiency of organic TE. The use of exfoliated BiTe nano-platelets [6] into polymer matrices will be studied for the first time. Moreover a particular emphasis will be given to the processability of these organic materials into forms and via processing routes compatible with industrial scale-up (extrusion, spinning, coating, etc.).

1. G.J. Snyder and E.S. Toberer, Nature Mater. 7, 105 (2008); **2.** N. Dubey, M. Leclerc, J Polym Sci Part B: Polym Phy, 49, 467–475 (2011); **3.** A. Khitun, A. Balandin, K.L. Wang. Superlattices Microstructures, 26, 181-193 (1999); **4.** O. Bubnova, Z.U. Khan, A. Malti, S. Braun, M. Fahlman, M. Berggren, X. Crispin. Nature Mater, 10, 429-433 (2011); **5.** D. Kim, Y. Kim, K. Choi, J.C. Grunlan, C. Yu. ACSNano, 4, 1, 513-523 (2010); **6.** Coleman, J. N et al.Science, 331, 568-571.

PLAN OF WORK

Activity	2	4	6	8	10	12	14	16	18	20	22	24	26	28	30	32	34	36	38	40	42	44	46	48 (month)
1.Project Management	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
2.Continuous Survey	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
3.Training				X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
4.Selection of Materials				X	X	X																		
5.Synthesis of Conductive Polymers					X	X	X	X	X	X	X	X												
6.Processing of Conductive Composites					X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X				
7.Preparation of Devices																					X	X	X	X
8.Characterisation & Evaluation							X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
9. Dissemination & Exploitation																					X	X	X	X
Milestone					M1											M2						M3		M4

The work is structured in nine activities, with 4 milestones and equivalent number of deliverables, as presented in the Gantt chart below:

Deliverables:

D1. Shortlist of conductive polymers and nanoparticles to focus on (Month 10).

D2. Preparation of TE polymers and composites, both n-type and p-type (Month 30).

D3. Preparation of TE devices (Month 29).

D4. Dissemination and Exploitation of results (Month 46).