Project Proposal Form – 2023 entry

Project Title	Engineering Flash Graphene for Novel Low-Cost Plastic Recycling Technology
University (where student will register)	University of Warwick
Theme (Max. 2 selections)	Climate & Environmental Sustainability ☒ Organisms & Ecosystems ☐ Dynamic Earth ☐
Key words	Plastic recycling; Flash graphene; nanographene; density functional theory; Plastic waste; sustainability
Supervisory team (including institution & email address	**PI: Dr Hatef Sadeghi** Hatef.Sadeghi@warwick.ac.uk **Co-I: Dr Soroush Abolfathi** Soroush.abolfathi@warwick.ac.uk

Project Highlights:

- Develop novel computational methodologies for multiscale modelling of formation of flash nanographene from plastic polymers
- Exploit a wide range of plastic polymers that can be recycled in the form of flash nanographene
- Identify plastic polymers that can be converted to nanographene with high recycling efficiency

Overview (including 1 high quality image or figure): *Maximum 350 words*

The production of non-fiber plastics between 1950-2017 has been estimated at 6789 million metric tons, and production is growing every year (Geyer et al., 2017). Much of the plastic is used for packaging, which becomes waste very quickly. Between 1950 and 2015, about 6300 million metric tons of primary and secondary (recycled) plastic waste was produced, of which only 9% was recycled, 12% was incinerated and 79% was deposited in waste dumps. Despite improvement in selective waste collection and less recyclable waste disposal to landfills, much of the plastic waste is still deposited in the environment.

Nearly all types of plastics are recyclable. However, the extent to which they are recycled depends upon technical, economic and logistic factors. Plastics are valuable resource, so the best outcome after their initial use is typically to be recycled into a new product. In recent years, many scientists have focused on developing effective and efficient methods to recycle plastic waste back into plastic polymers, solvent, oil or other chemical components. It was demonstrated recently that by flash Joule heating of inexpensive carbon sources such as rubber tyres and mixed plastic waste, plastic could be recycled to carbon allotropes (Luong, et al. 2020). This ground-breaking method can recycle plastics into graphene in a very fast process which takes less than a second. The product, named flash graphene (FG) after the process used to produce it, shows turbostratic arrangement (that is, little order) between the stacked graphene layers.

FG synthesis is a sustainable method for plastic recycling without the need for purification steps and uses no furnace and no solvents or reactive gases. The electric energy cost for FG synthesis is only about 7.2 kilojoules per gram, which could render FG suitable for use in bulk composites of plastic, and other carbon-based materials. So far, little is known about the underlying mechanism of formation of flash graphene. This PhD project aims to develop novel methodology to model formation of flash nanographene from plastic polymers and to develop the scientific understanding necessary to optimise the formation process and identify plastics that can be converted to nanographene efficiently.

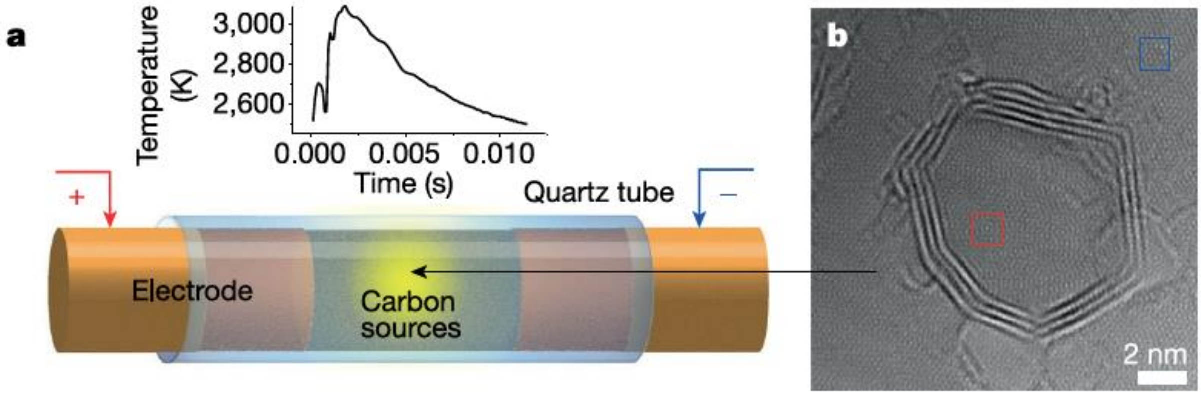

Figure 1: (a)Schematic of the Flash Joule Heating process, and plot of the temperature rise versus time during flashing. (b) image of Carbon Black-Formed Graphene on top of a single layer of coffee-derived Flash Graphene. (adopted from Loung et al., 2020)

Methodology: *Maximum 150 words*

This PhD will predominantly focus on developing novel numerical modelling tool capable of simulating flash nanographene formation from a range of plastic polymers providing an insight into what kind of plastic waste are the most appropriate for such recycling and how the recycling process can be scaled up and optimized. We will use Molecular Dynamic Simulation to study the dynamic of formation of nanographene from plastic polymers combined with density functional theory (DFT) and tight-binding DFT for their mechanical and electronic properties.

Training and skills: *Maximum 100 words – excluding CENTA training information*

Students will be awarded CENTA2 Training Credits (CTCs) for participation in CENTA2-provided and 'free choice' external training. One CTC equates to 1⁄2 day session and students must accrue 100 CTCs across the three years of their PhD.

Training will be provided in a wide range of numerical and analytical tools needed to simulate flash nanagraphene formation processes. Supports will be provided to help design and develop the numerical model to study the behaviour of different plastic polymers in the recycling process. The student will be trained on cutting edge atomistic scale numerical modelling techniques for simulation of nanomaterials using molecular dynamic and density functional theory. Through our industrial partners a range of training activities will be provided on plastic waste management methodologies and challenges, recycling technologies and their efficiency/added value, plastic pollution risk management, as well as, communication and public understanding of science. In addition, the student will be able to work closely with plastic recycling and synthesis scientists and creation team, ensuring that their science will be applied and tested at full industrial scale.

Partners and collaboration (including CASE):

Name of L1/L2 Partner (where applicable)	

Name of CASE partner (where applicable – project proposal **must** be accompanied by a letter of support from the CASE partner)	*Environmental Sustainability Associates Limited* *MURA Technology*

Further information on partners and collaboration (including CASE): *Maximum 100 words*

This PhD project benefits from supervision by two internationally leading research groups at the University of Warwick including, Warwick Water Group and the Centre for Predictive Modelling at the School of Engineering. The research team of this project are internationally recognized for their research into the plastic waste impacts on the environment and simulation of nanoscale materials. Besides the standard NERC PhD funding, the project is supported by UKRI Future Leaders Fellowship number MR/S015329/2, and the 'Garbage In, Value Out' project funded by the UK Foreign and Commonwealth Development Office. The Student will have the opportunity of working closely with the research end-user and industrial collaborators. Furthermore, there will be internship and placement opportunity for the student at the *Environmental Sustainability Associates Limited* and *MURA Technology* to engage with a range of related projects in plastic waste management, plastic recycling technologies and challenges, communication and public understanding of science and plastic pollution risk management.

Respiratory and Contact Infection Resilience of the Project: *Maximum 100 words:*

Given that this PhD is predominantly focusing on numerical modelling investigations, COVID19 will not have a notable effect on the project and the student progress. The supervisory meetings will be hold online and access to all computational resources (PC, HPC, etc.) will be given through VPN secure connections.

Possible timeline:

Year 1: Basic research skill training; literature review and familiarisation with atomistic simulation methods and analysis techniques and development of computational methodology for simulation of formation of nanographene from plastic polymers

Year 2: Comprehensive numerical modelling of flash graphene formation for a range of plastic polymers. Investigating the impacts of particle density, size and shape on the efficiency of nanographene formation.

Year 3: Detailed analyses of numerical data to identify the classes of plastic polymers that can be converted to nanographene with high recycling efficiency. Writing the thesis will take place during the final year.

Further reading: (*in Harvard Reference Style*)

Journal:

Geyer, R., Jambeck, J. R., Law, K. L. Production, use, and fate of all plastics ever made. Science Advances, Vol. 3, No. 7, e1700782 (2017). DOI: 10.1126/sciadv.1700782

Luong, D.X., Bets, K.V., Algozeeb, W.A. et al. Gram-scale bottom-up flash graphene synthesis. Nature 577, 647–651 (2020). DOI: 10.1038/s41586-020-1938-0

Sadeghi, H. Theory of Electron, Phonon and Spin Transport in Nanoscale Quantum Devices, Nanotechnology, 29 (37), 373001 (2018). DOI: 10.1088/1361-6528/aace21

Further details:

Further details about the supervisory team of this project can be find here:

Dr Hatef Sadeghi: https://warwick.ac.uk/nanolab

Dr Soroush Abolfathi: https://warwick.ac.uk/fac/sci/eng/staff/sa/

Further information about Warwick Centre for Predictive Modelling can be found here:

https://warwick.ac.uk/fac/sci/wcpm

Further details:

For any inquiry related to this project please contact Hatef.Sadeghi@Warwick.ac.uk and Soroush.Abolfathi@Warwick.ac.uk