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Experiment and theory to inform industrial graphene manufacturing: Building up the Materials Genome

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14. ABSTRACT
The purpose of this study was to address mechanical deformation of 2D systems to later correlate with device performance and improve fabrication. Our group has reported innovative approaches to fundamentally characterize effects of fabrication and processing on rippled and strained graphene on a quantitative level, with molecular sensitivity, at wafer scales. This approach has merged state of the art synchrotron hyperspectral detectors with advanced theoretical calculations and data analytics. Looking forward, this effort will gain from the addition of expertise in the realm of data analytics and artificial intelligence (AI).

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Experiment and theory to inform industrial graphene manufacturing: Building up the Materials Genome

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Investigation of surfaces and nano-interfaces through advanced microscopies and spectroscopies: theory, experiment, and data.

Background

The incipient field of 2D materials, inclusive of graphene, holds promise in a multiplicity of scenarios, despite drawbacks. Namely those are lack of band gap as well as poor manufacturing technologies that do not comply with standard microtechnology practices. In collaboration with the Grote team at Wright Patterson Air Force Laboratory, we have developed an innovative approach, combining experimental and theoretical NEXAFS spectroscopy to address these issues in the context of graphene, which is extendable to other 2D systems. The purpose of this study was to address mechanical deformation of 2D systems to later correlate with device performance and improve fabrication.

Contributions from prior AFOSR funding

Prior/current AFOSR funding and cost sharing (see Annex) has yielded a number of contributions in the realm of surfaces and nano-interfaces in materials systems of great interest to AFOSR (see Annex and Bibliography). Indeed, The Laboratory for Matter Dynamics (LMD) has demonstrated extensive expertise in the analysis of interfaces in soft matter under acknowledged AFOSR funding. [1-4]

Contributions from Current AFOSR Award

Recently, our group has reported innovative approaches to fundamentally characterize effects of fabrication and processing on rippled and strained graphene on a quantitative level, with molecular sensitivity, at wafer scales. These results are discussed in two publications that acknowledge current AFOSR award [5-6]. This approach has merged state of the art synchrotron hyperspectral detectors (NIST-Brookhaven National Lab) with advanced theoretical calculations (Molecular Foundry-Lawrence Berkeley National Laboratory) and data analytics (Stanford Linear Accelerator). Looking forward, this effort will gain from the addition of the expertise at U. Maryland in the realm of data analytics and artificial intelligence (AI), as shown in a recent co-authored publication. [7]

Future work and Interest to AFSOR

This project is highly innovative as it pioneers the study of graphene Microtechnologies through the new generation of hyperspectral detectors, as well as the analysis of graphene technology through a Materials by Design paradigm. This topic is highly relevant to AFOSR towards biosensing and soldier health monitoring wearable technologies, amongst others. This project is also game changing in the realm of Big Data, as it will produce metrology standards towards the

optimum fabrication of both graphene devices and structural composites while increasing and leveraging efforts in photonics at international levels.

The wealth of information embedded in hyperspectral imaging has promoted the construction of a theoretical database of graphene defects that, through AI routines, will be able to mine data to produce qualitative and quantitative analysis and hence, information about the overall quality of graphene.

It is worth emphasizing that these approaches have overall, the feasibility of being deployed in a number of systems of high technological interest, such as nanotubes, 2D materials, and MXenes.

Indeed, the renowned expertise in the analysis of C-K edge by NEXAFS-synchrotron spectroscopies is promoting other groups to reach out in the spirit of collaborative work, hence the intention to further this effort.

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Selected Posters:

1. "Simulations of NEXAFS to study processing effects on Graphene" at Ninth York Doctoral Symposium on Computer Science & Electronics University of York, York, UK. 2016
2. "X-ray Absorption Spectroscopy study of processing effects on Graphene: Experiment and Theory" at Molecular Foundry User Meeting Lawrence Berkeley National Laboratory, Berkeley, CA, USA. 2016

ANNEX

Prior/current AFOSR funding and cost sharing

An introductory travel grant from the Air Force Office of Scientific Research in 2012 awarded to Professor Campo (Window on Science) later derived in an ongoing program: FY14 ($29.2 K FA9550-14-1-0099), and FY15 ($50k, FA9550-15-1-0289). Recently, in FY16 a **AFOSR Director's Award** has been granted ($41k, FA9550-17-1-0082) following the same research theme, first started in collaboration with the Grote Group at Wright Patterson, titled "Experiment and Theory to Inform Industrial Graphene Manufacturing: Building Up the Materials Genome"**.**

Synergistic funding: White House Office of Science and Technology Policy May 5-6 2014 ($ 2k), NSF-Institute for Pure and Applied Mathematics- UCLA, July 21 – August 1, 2014 ($ 2k), and Fujitsu-HCPW *Fellowship towards a Ph.D. student* (£ 75K). Additional US Government Agencies Funding: DOE SC Programs: BES and ERRE, amongst other under Contract Nos. DE-AC02_98CH10886, DE-AC02-05CH11231, and NIST SBIR Phase III under ARRA Funding NIST SB134109SU1067 (BNL, LBNL, and Synchrotron Research respectively). EU funding supported HPCW: ERDF 2007 – 2013 Project No. 80621. UTSA and SLAC have also provided in kind funding through the use of facilities and personnel's time.