

## **AFRL-AFOSR-JP-TR-2023-0063**

3D printing of 2D (two dimensional materials) for robust electronics

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**Standard Form 298** (Rev.5/2020) Prescribed by ANSI Std. Z39.18

Name of Project: Printing of 2D (Two Dimensional) Materials for Robust Electronics

Sanction Letter No & Date:FA2386-19-1-4039, Proposal-19IOA039,Dt.02-05-2019

Duration of the Project:3years

Principal Investigator of the above Project: Prof. Chandra Sekhar Tiwary,

Department of Metallurgical and Materials Engineering, IIT Kharagpur

## Highlight of the project

Followings are the results from project which were highlighted as cover-page in different journals

# **Nanoscale**



**EXECUTE BARBEL COMMANDER AND THE SECOND PROPERTY**<br>OF CHEMISTRY **COMMANDER COMMUNISTIES** 

Atomically thin Cobalt telluride was used in electronics gazettes, to collect energy from waste heat. Waste heat and small mechanical pressures are used by buildings covered in cobalt telluride to create energy and light the city. We describe how 2D cobalt telluride's combination piezoelectric and triboelectric capabilities can be used to produce energy from waste heat in this article  $(CoTe<sub>2</sub>)$ . A five-fold increase in energy conversion efficiency was achieved by the piezo-triboelectric nanogenerator, which generated an open-circuit voltage of ~5V when subjected to a 1 N force. With a maximum voltage of about 10 V, a quick response time, and high responsiveness, the 2D piezo-tribogenerator has exceptional qualities.

Nanoscale, 2022,14, 7788-7797, https://doi.org/10.1039/D2NR00132B



Compared to conventional treatment methods, 3D printed materials with configurable surface area, thickness, and roughness improve the removal effectiveness of heavy metals, oil, and organic matter from water.

Advanced Sustainable Systems, 2022, https://doi.org/10.1002/adsu.202100282







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In this study, we gather and organise data on a broad range of 2D tellurides. The review seeks to give a general understanding of the materials' synthesis techniques, characteristics, and uses. We list numerous binary tellurides and talk about the fascinating characteristics that arise when a third element is added. Our investigation includes the optical, electrical, photo-electrochemical, magnetic, and quantum aspects of these 2D layered materials. Finally, we discuss future directions for this study as well as issues that must be resolved in order to fully realise the potential of 2D tellurides in a wide range of applications.

Materials Today, 2021, 402-426, https://doi.org/10.1016/j.mattod.2021.08.008

We present the pulsed laser ablation of electronic trash in deionized water for the manufacture of high-quality functional graphene from one of the main parts of e-waste, the polymeric component. Systematic modelling identifies the ideal laser parameters for the maximum yield of  $~10\%$  and good-quality graphene. For highly conductive electronics contacts that will be useful for upcoming robust electronics applications, high-quality synthetic graphene has also been used.

ACS Sustainable Chem. Eng. 2021, 14090–14100, doi.org/10.1021/acssuschemeng.1c03817

Topologically engineered 3D printed architectures with superior mechanical strength. Gyroids, Menger cubes, and origami/kirigami-based constructions are a few examples of quite unusual structures that have developed from advanced geometrical concepts. In other cases, innovation has resulted from emulating nature in bio-inspired materials (e.g. honeycomb structures, nacre, fish scales etc.). Using computer-aided design models, additive manufacturing has made it possible to easily fabricate complicated geometrical and bio-inspired architectures. These structures' mechanical qualities, including as strength, stiffness, and toughness, have been improved through the use of simulations and tests. In this paper, we give

an overview of topologically designed materials with ideal mechanical properties that are also easily printable via additive manufacturing.

## Materials Today, 2021, 72-94, https://doi.org/10.1016/j.mattod.2021.03.014



Energy Harvesting from Atomically Thin  $Co<sub>2</sub>Te<sub>3</sub>$ . The liquidphase exfoliation technique is used to successfully exfoliate 2D  $Co<sub>2</sub>Te<sub>3</sub>$  from the bulk crystal  $Co<sub>2</sub>Te<sub>3</sub>$  as it was manufactured. It is discovered that the exfoliated  $Co<sub>2</sub>Te<sub>3</sub>$  is a weakly ferromagnetic semiconductor material. With an output voltage of about 3.6 V, 2D  $Co<sub>2</sub>Te<sub>3</sub>$  is also employed as a nanogenerator employing the flexoelectric effect. The ability to harvest energy was also studied at room temperature under various magnetic fields. Our density functional theory calculations confirm the magneto-crystalline anisotropy of this 2D monolayer system, and provide a microscopic insight into origin of the electric response under a magnetic field. Such electric response in atomically-thin material is particularly desirable for

applications in nanoscale devices.

## J. Phys. Chem. C 2022, https://doi.org/10.1021/acs.jpcc.2c02102



In this study, liquid-phase exfoliation from the naturally common mineral biotite is used to demonstrate the synthesis and characterisation of the ultrathin metal oxide known as biotene. The flexoelectric property of atomically thin biotene is utilised for energy harvesting by repeated bending. Surface charges cause a rise in the effective flexoelectric response, leading to voltage increases of up to 8 V and a high mechano-sensitivity of  $0.79$  V N<sup>-1</sup> for normal force. Simulations using the density functional theory (DFT) serve to confirm this flexoelectric response. The magnetic field and thermal heating respond more strongly to the atomically thin biotene. A variety of potential two-dimensional (2D) oxide materials for energy production and energy harvesting applications are predicted by the synthesis of the metal-oxide twodimensional (2D) biotene.

Small 2022, 2201667, https://doi.org/10.1002/smll.202201667

The key objectives of the projects :

- I. Synthesis of high-quality large scale 2D materials
- II. Preparation of 2D materials-based gel/liquid for printing
- III. Engineering 3D printer for printing of 2D materials
- IV. Printing high surface area, strong, robust architecture of 2D materials using 3D printer
- V. Post processing of the interconnected architecture
- VI. Building understanding and know-how using materials simulation

## Deliverables

The project deliverables are divided into three sections. A. Synthesis of large scale 2D materials and their ink; B. Engineering 3D printer and optimize topology to make architectures with high strength, low density and high surface area; C. Decorating the 3D printed structures with 2D materials D. Printing using the 2D materials

We have optimized the process for synthesis of high quality and large scale 2D materials, nanoparticles. Simulation based optimum concentration of mixture for printing different components has been done in the project. The 3D printer is developed/modified for 3D printing of 2D materials.

We have produce well characterize 2D with metal and oxide nanoparticle. The liquid gel of chemically interconnected hybrid with required viscosity for 3D printing is produce. 3D printing of the 3D architecture using 2D materials gel. Mechanical and physical testing of the architecture. Testing of the 3D architecture for pollutant adsorption.

The results of the project are divided in subsequent sections and publication is cited as well



Conducting Graphene Synthesis from Electronic Waste, ACS Sustainable Chem. Eng. 2021, https://doi.org/10.1021/acssuschemeng.1c038  $17$ 



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Shear exfoliation synthesis of large-scale graphenereinforced nanofibers, Carbon, 166, 2020, 405-413

Extraction of Two-Dimensional Aluminum Alloys from Decagonal Quasicrystals, ACS Nano 2020 14 (6), 7435-744



Scalable Synthesis of Atomically Thin Gallium Telluride Nanosheets for Supercapacitor Applications, ACS Appl. Nano Mater. 2021, 4, 5, 4829-4838



Green Route for Beneficiation of Metallic Materials from Electronic Waste for Selective Reduction of CO<sub>2</sub>, ACS Sustainable Chem. Eng. 2020, 8, 32, 12142-12150



decorated p-type 2D-molybdenum disulfide (MoS2) for enhanced hydrogen sensing, Nanoscale, 2020,12, 11830-11841

Entropy Alloys: Assisting the Oxygen Evolution Reaction at the Thermodynamic Voltage, ACS Catal. 2021, 11, 14000-14007, https://doi.org/10.1021/acscatal.1c03571

Formic acid and methanol electro-oxidation and counter hydrogen production using nano high entropy catalyst, Materials Today Energy, 16, 2020, 100393

#### Preparation of ink for 3D printing template



Improved mechanical and wear properties of Cu-Ga-In ternary alloys through liquid reinforcement, Materials Today Communications, 27, 2021, 102409



Probing the bacterial detoxification of cadmium to form cadmium sulfide quantum dots and the underlying<br>mechanism, Mater. Adv., 2020,1, 1168-1175



Bioinspired Aluminum Composite Reinforced with Soft Polymers with Enhanced Strength and Plasticity, Adv. Eng. Mater., 2020, 22: 1901116.



Hexagonal boron nitride-carbon nanotube hybrid thermal, network structure for enhanced mechanical and electrical properties of polyimide nanocomposites. **Composites** Science and Technology, 188, 2020, 107977

#### **Preparation of 3D printing template**



Deformation resilient cement structures using 3D-printed molds, iScience, 24, 3, 2021, 102174



On the mechanical properties of atomic and 3D printed zeolite-templated carbon nanotube networks, Additive Manufacturing, 37, 2021, 101628



Flexure resistant 3D printed zeolite-inspired structures, Additive Manufacturing, 47, 2021, 102297



Atomic Scale Structure Inspired 3D-Printed Porous Structures with Tunable<br>Mechanical Response, Adv. Eng. Mater., 23:2001428., 2021





Understanding the mechanics of complex topology of the 3D printed Anthill architecture, Oxford Open **Materials** Science,  $2,$ 2022, https://doi.org/10.1093/oxfmat/itac00  $\mathsf 3$ 

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#### **Applications of 3D printing structures**



Development of a schwarzite-based moving bed 3D printed water treatment system for nanoplastic remediation, RSC Adv., 2021, 11, 19788-19796



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Emerging 2D metal oxides and their applications, Materials Today, 45, 2021, application



Review of strategies toward the development of alloy two-dimensional (2D) transition metal, iScience, 24, 103532, 17, 2021, https://doi.org/10.1016/j.isci.2021.103532



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Atomically thin gallium telluride nanosheets: A new 2D material for efficient broadband hew 2D material for emteric broadcar<br>nonlinear optical devices,<br>Appl. Phys. Lett. 120, 021101 (2022);<br>https://doi.org/10.1063/5.0073205



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## Lab facilities developed using project



## Student trained during the project



## Meeting organized through the project

Several online meetings were organized with AFRL team.

Two Meetings at IITKGP were organized