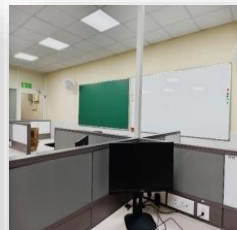




সিএসআইআর-কেন্দ্রীয় কাঁচ ও সেরামিক গবেষণা সংস্থা
सीएसआईआर-केंद्रीय काँच एवं सिरामिक अनुसंधान संस्थान
CSIR-Central Glass & Ceramic Research Institute
"Innovation in Ceramics and Glass for mankind"



Information Technology & Computational Materials Section
CSIR-CGCRI, 196 Raja S. C. Mullick Road
Kolkata-700032

Overview

Research Areas

- ▶ Multiscale modelling: DFT, MD, and FEA
- ▶ Functional and sensing properties of layered structures
- ▶ AI-driven accelerated glass discovery
- ▶ Generative AI for molecular dynamics trajectory sampling
- ▶ Graph Neural Network-based plasticity and failure analysis
- ▶ ML predictive capability for additive manufacturing processes
- ▶ Engineering design and structural optimisation framework
- ▶ Unified computational Design Centre for CGCRI community

National Missions & SDGs

4 QUALITY EDUCATION



7 AFFORDABLE AND CLEAN ENERGY



9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



12 RESPONSIBLE CONSUMPTION AND PRODUCTION



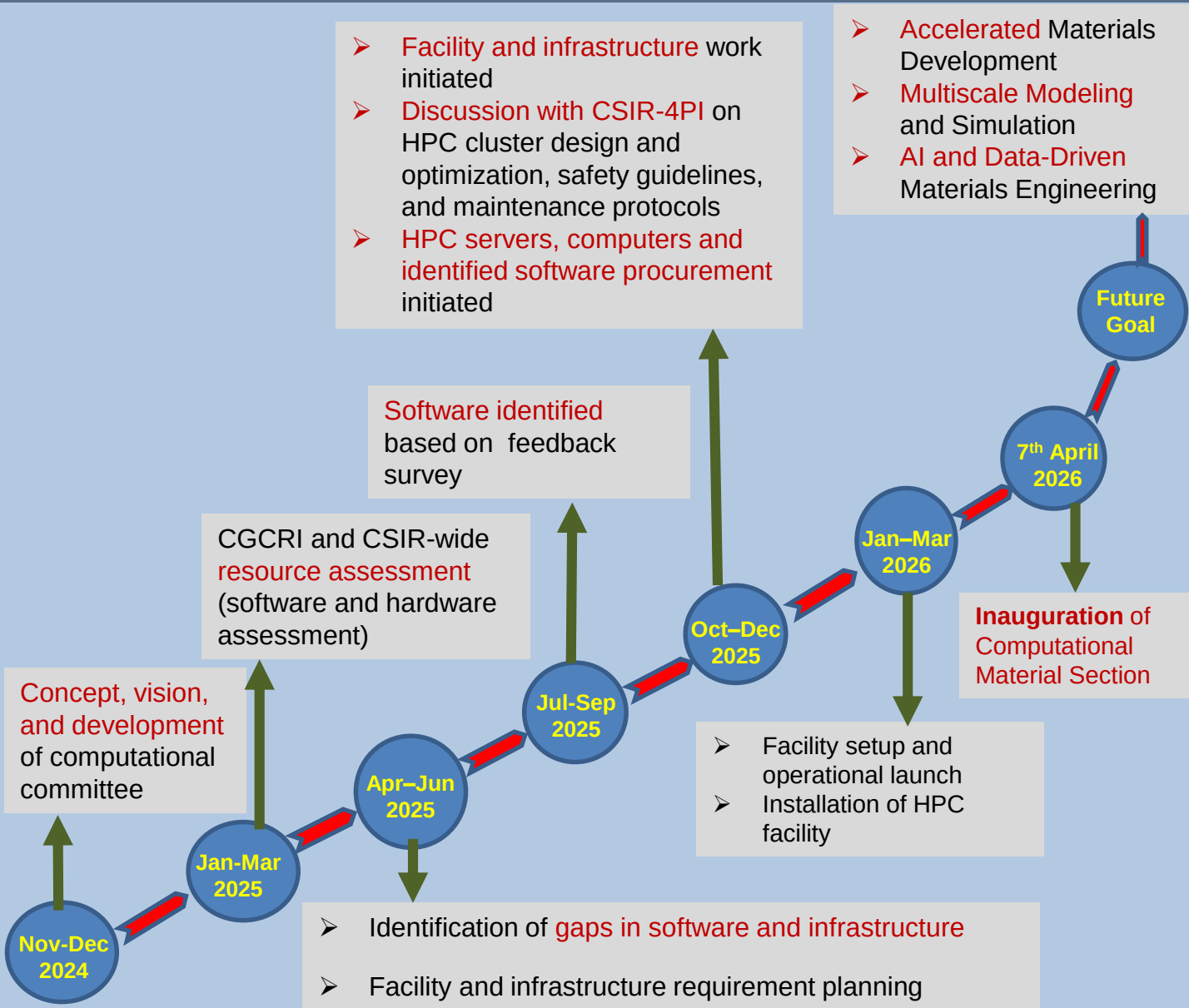
Mission & Relevance

Mission: To unify fragmented computational research efforts at CSIR-CGCRI into a collaborative platform that empowers young researchers, establishes shared resources, and drives programs of significant scientific and national relevance.

Relevance: The section integrates multiscale modelling, AI and data-driven methodologies, and advanced computational frameworks to bridge fundamental atomic-scale understanding with accelerated materials discovery, functional property prediction, and engineering design — establishing a comprehensive computational ecosystem for next-generation ceramic, glass, and advanced material development of industrial and national relevance.

The Information Technology and Computational Materials Section is committed to a comprehensive research paradigm — from fundamental atomic-scale investigations to AI and data-driven accelerated discovery — aimed at developing novel functional materials with direct industrial and technological relevance.

▶ Roadmap of Computational Materials Section



The Team

Scientist



Development of web applications and database management systems, Laboratory

Mr. Jyotirmay Sikder, HOD



Statistical physics, Computational material science, Machine learning-driven functional material design

Dr. Indrajit Tah



Crystallography, electron-density, structure-property relations, gas sensing, phase-change material applications

Dr. Swastik Mondal



Computational materials science using VPSC, FEM and TEM simulation

Dr. Soupitak Pal



Biomechanics, implant design, finite element analysis, biomaterials, AI-driven additive manufacturing

Mr. Ankush Pratap Singh



FPGA-based neuromorphic smart vision and gas sensors for multifunctional applications

Dr. Subhajit Das

Emeritus Scientist



Computational Chemistry in Drug Design, Biomolecular Sensing, and Materials Science

Dr. Bishwajit Ganguly

Technical Staff



Agniv Adhikari



Unmona Sikdar



Md. Sharif



Kalyan Das



Abhishek Mukherjee



Sukanta Basak

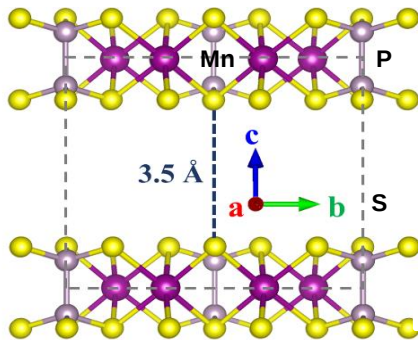


Mr. Himanshu Gupta

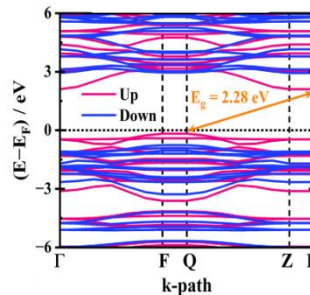
Research Theme

First-Principles Electronic Structure Calculations for Gas Sensing Applications and Quantum Material Design

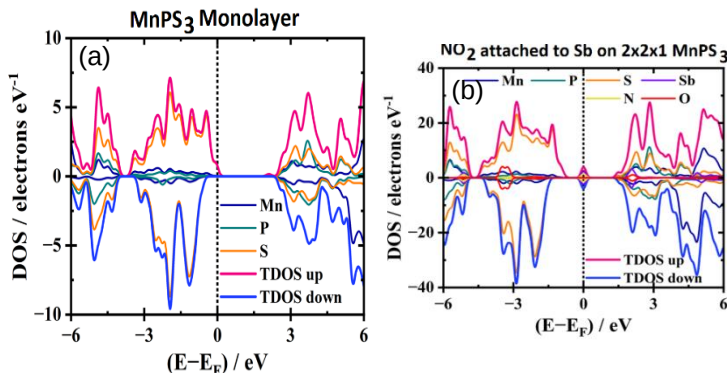
Can *p* block elements act as SACs? – First principles calculations involving DFT+*U* are invoked to answer this



MnPS₃ optimized structure

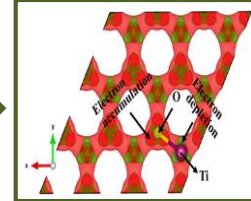
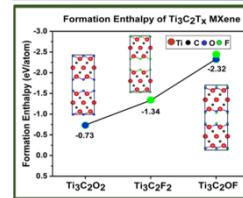


Spin-polarized electronic band-structure - monolayer

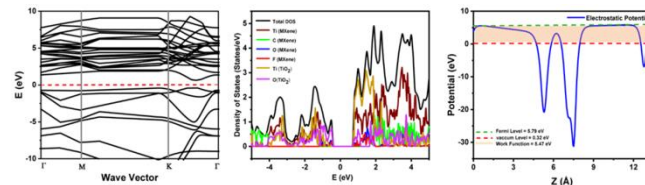


Total and projected density of states: (a) without and (b) with Sb-NO₂

Integrated DFT-ML framework for MAX phase and 2D-MXene design

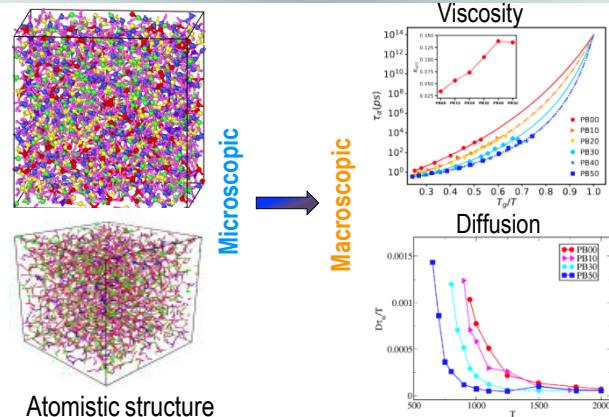


Structural stability of MXene with charge neutrality



Band gap, DOS and Work-function of MXene

From Atomic Scale to Engineering Properties in Materials Science



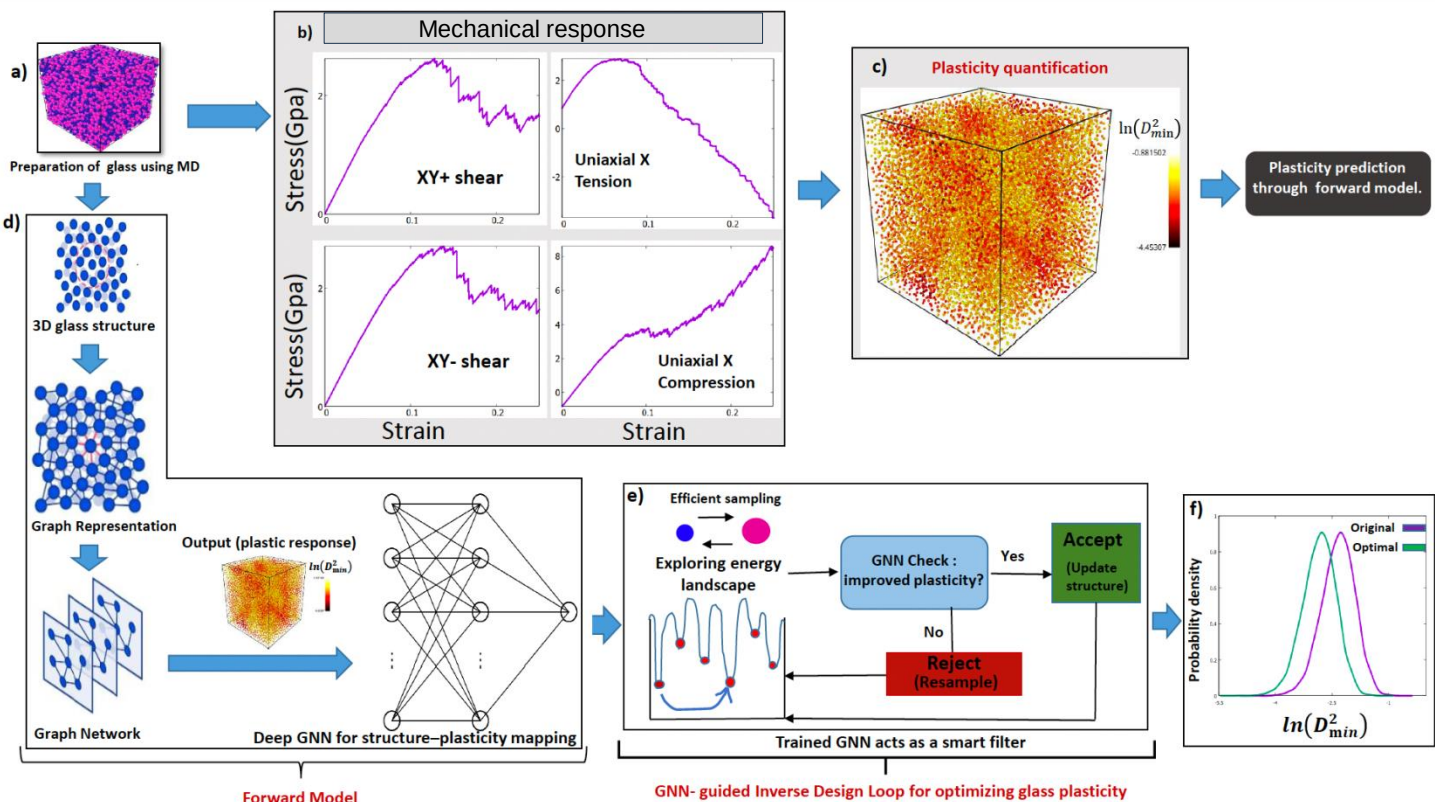
- Gas sensing
- Molecular Dynamics

- Monte Carlo
- Biomolecular Sensing

- Integrated DFT-ML framework
- Microstructure Engineering

Research Theme

AI-driven Inverse Design of disorder materials with targeted plasticity



- Mechanical response

- Microstructure generation

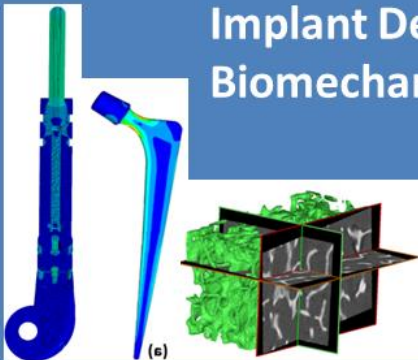
- Physics informed ML

- Inverse Design

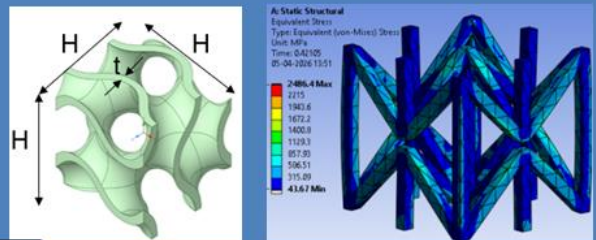
Research Theme

Finite Element and Computation fluid dynamics analysis for engineering application

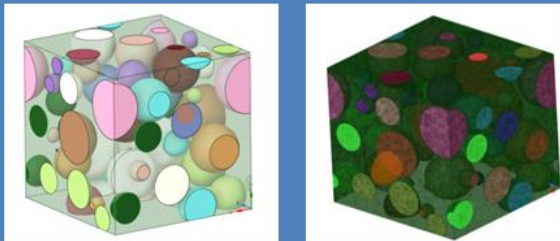
Implant Design & Biomechanics



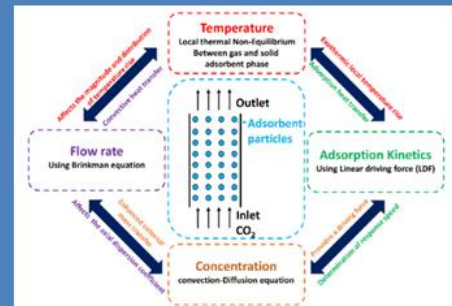
Designing lattice structures



Microstructural Modelling



Multiphysics simulation

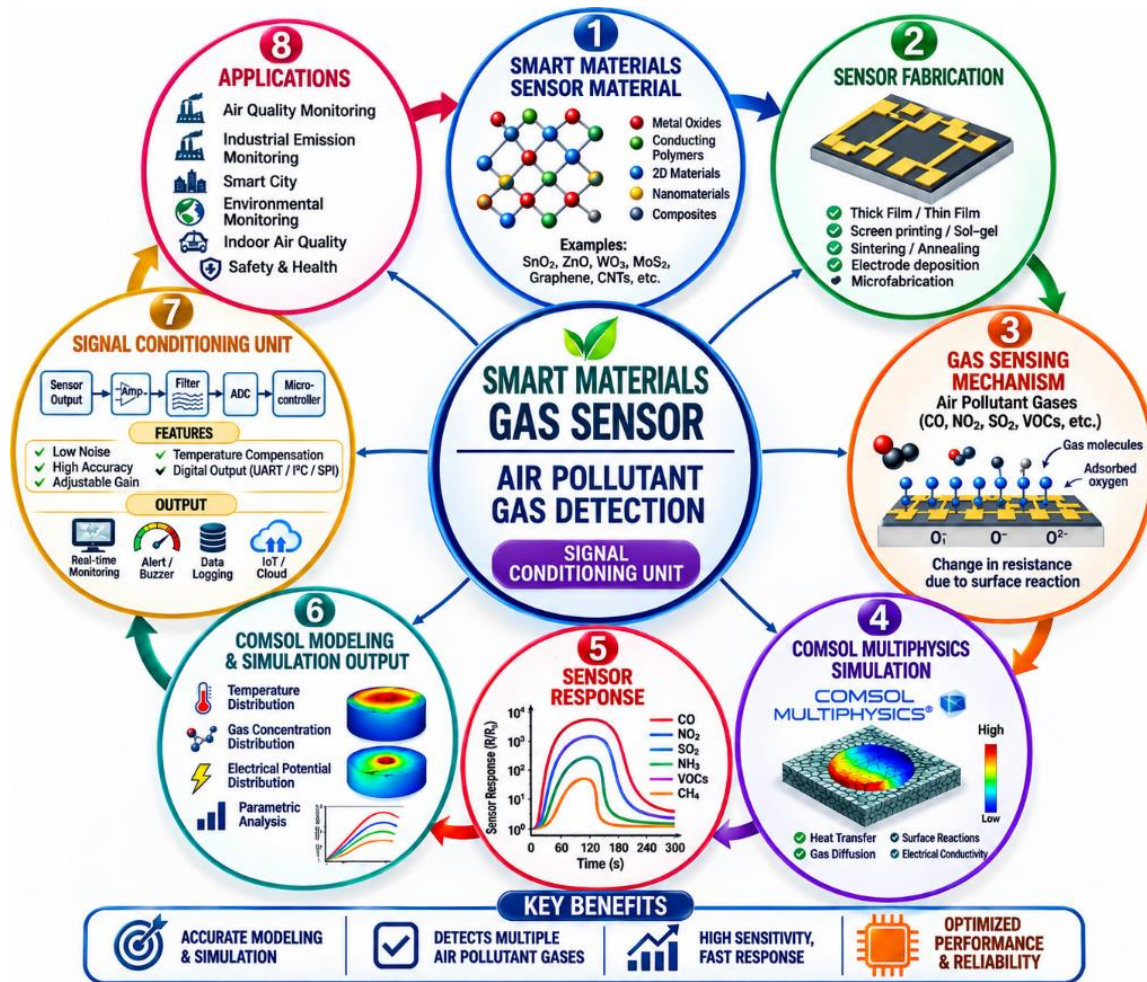


- FE & CFD Analysis
- Microstructural Modelling

- Lattice Structure Design
- Multiphysics Simulation

Research Theme

Simulation and Development of Smart Materials based Gas Sensors



- Materials Informatics
- Intelligent Sensor Systems

- Predictive Modeling
- Smart Materials

R&D Facilities

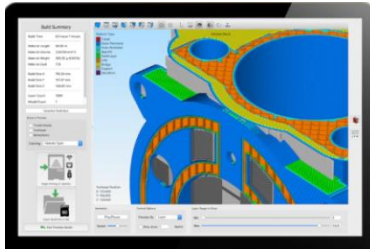


**Shared Computational Facility
“ANANT” & “CHAMP” at CSIR-
NIDSAI**

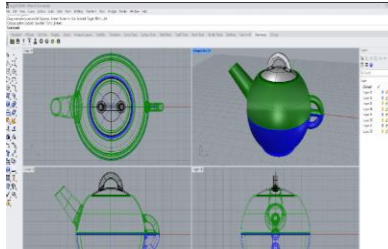


Dedicated Local computing facility

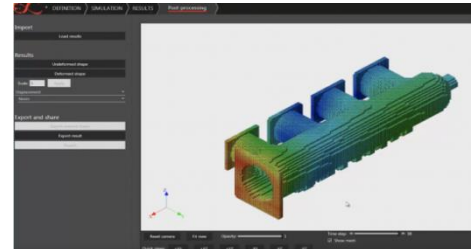
Software



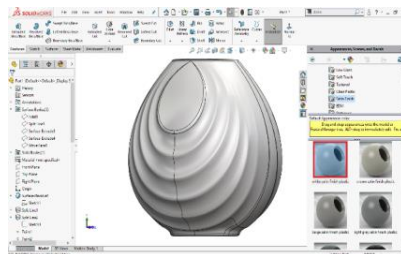
Simplify 3d



Rhino 3d



Digmat-AM



Solidworks



Materise Mimics



R&D Projects

- **Multifunctional Mechanical Metamaterial for Life Support in Manned Submersibles**, funded by Ministry of Earth Science under deep ocean Mission (November 2024 – October 2026) **Funding:** 115.7 Lakhs
- **Design Glasses with tailored properties (e.g., high hardness with low weight) for industry and societal need**, funded by CSIR under CLAIM Mission (June 2025 – March 2028) **Funding:** 111.37 Lakhs
- **In-silico study to unravel the electronic and structural effects of semiconductor metal oxides to augment the selectivity for gas sensing in real environmental conditions** funded by CSIR HRDG EMR2 (2026 – 2029) **Funding:** 37.34 Lakhs
- **Development of chemiresistive ceramic-polymer nanocomposites for food spoilage detection at sub-ambient temperature** CRG project sponsored by SERB/ANRF (March 2025 – March 2027) **Funding:** 47.91 Lakhs
- **Development of Quantum Materials and Photonic Platforms for Quantum Technologies (WP01: Development and Identification of Stoichiometric Alkaline-Earth-based Quantum Materials as Superconducting Platforms)** funded by CSIR under RDSF (April 2026 – March 2027) **Funding:** 20 Lakhs
- **Development of sol-gel derived zirconia short fiber for high temperature ceramic matrix composite**, funded by ASL, DRDO (Jan 2025 – Jan 2028) **Funding:** 96.26 lakhs

Key Stakeholder



Technologies under Development

SIGMA

Scientific Intelligence in Glass Materials & Applications

SIGMA: A web platform to search, visualize and predict glass properties

A database consists of **250K** glass composition and **300** glass Properties.

 **Search a Composition**
Find glasses by oxide makeup

1 **Pick an oxide**
from the periodic table/ by its name
Pick the properties

2 **It's added**
chip shows in your list

3 **Set a range**
min / max weight % (optional)

4 **See the results**
matching glasses appear

 **Visualize the Data**
Plot and explore results

1 **Choose a plot**
XY graph or ternary triangle

2 **Set the axes**
pick what to compare

3 **Adjust the view**
scale, colour, 2D or 3D

4 **Chart appears**
with a live point count

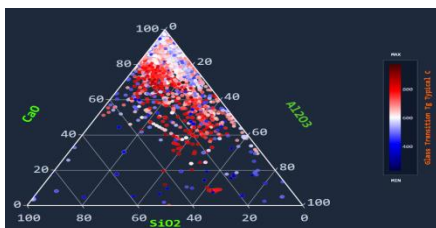
 **Predict a Property**
Let the model estimate values

1 **Choose a property**
e.g. Refractive Index

2 **Add your oxides**
set % (must total 100)

3 **Hit Predict**
sent to the AI model

4 **Get the answer**
value + composition profile

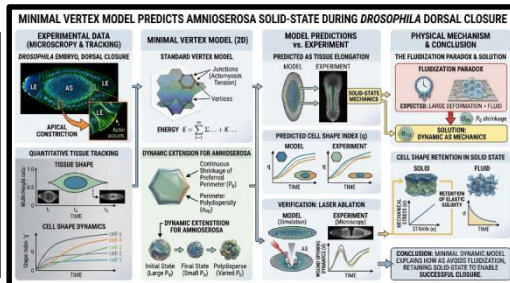


Key Publications

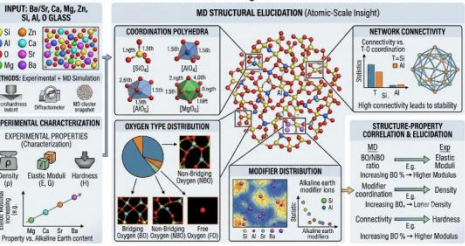
Minimal vertex model explains how the amnioserosa avoids fluidization during *Drosophila* dorsal closure.

Proceedings of the National Academy of Sciences, USA, 122, (2024)

By incorporating dynamic cell perimeter shrinkage, this extended vertex model explains how *Drosophila* amnioserosa tissue avoids fluidization and remains solid during dorsal closure. The framework successfully predicts experimental tissue behavior validated by live-imaging and laser ablation.



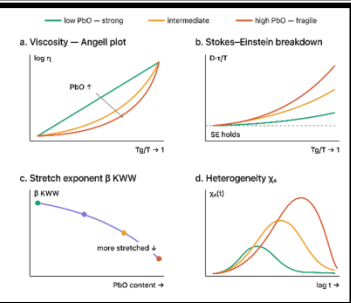
STRUCTURE-PROPERTY CORRELATION IN Ba/Sr-Ca-Mg-Zn-Si-Al-O GLASS: EXP + MD ELUCIDATION



Structure-Property Correlation in Ba/Sr-Ca-Mg-Zn-Si-Al-O Glass: Elucidation by Experimental and Molecular Dynamics Simulation Study

The Journal of Physical Chemistry B 128 (49) (2024)

This study combines MD simulations with experiments to reveal how substituting alkaline earth modifiers alters the glass network structure. It demonstrates that barium and strontium additions optimize bridging oxygen distribution and atomic connectivity, directly enhancing the material's mechanical hardness, density, and elastic moduli.



Tuning Fragility in Sodium Lead Borate Glasses: Unveiling the Interplay Between Compositions, Stokes-Einstein Breakdown, and Dynamical Heterogeneity

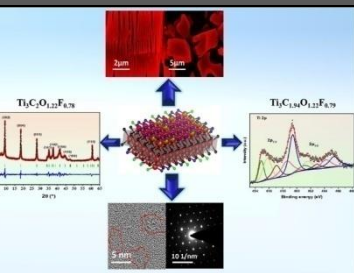
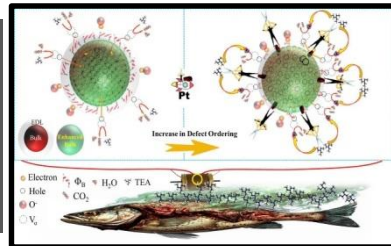
The Journal of Chemical Physics 164 (12) (2026)

Four panels, one color code (teal → amber → coral = increasing PbO):
(a) Angell plot bends from Arrhenius to super-Arrhenius **(b)** Stokes-Einstein product stays flat for strong, rises sharply for fragile. **(c)** β_{KWW} falls with PbO - relaxation more stretched. **(d)** χ_4 peak grows and shifts later - stronger dynamical heterogeneity.

Defect-ordered γ -Fe₂O₃-Pt interfaces governing amine adsorption and charge transfer: insights from rietveld, XPS, and DFT studies

Applied Surface Science, 741, 167159 (2026)

Sonochemically synthesized 3 wt% Pt- γ -Fe₂O₃ detects triethylamine down to 200 ppb with ~1.9 s response, excellent selectivity and stability, with first-principles calculations linking performance to cation-vacancy defect engineering



Multimodal characterization of near accurate surface chemistry and structural model of 2D-Ti₃C₂T_x MXene

Applied Surface Science Advances, 34, 101028 (2026)

A new Ti₃C₂T_x structural model with randomly distributed O/F terminations (~84%/16%) is proposed, which determines MXene surface chemistry self-consistently via XRD, XPS, PDF, and first-principles analysis, enabling reliable large-scale quality control.

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CSIR-Central Glass & Ceramic Research Institute
"Innovation in Ceramics and Glass for mankind"



ITCMS



A Kaleidoscope of Eras



Women's Compendium



Safety Manual



Technology Compendium



How to Reach Us

Contact

General Enquires: pro.cgcri@csir.res.in

Scientific & Technological: pmd.cgcri@csir.res.in