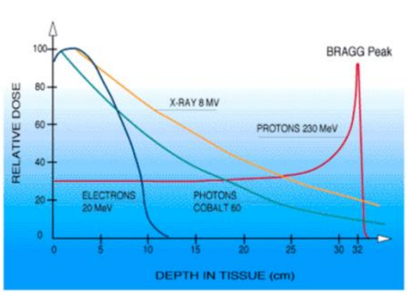
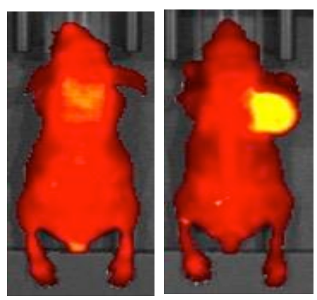
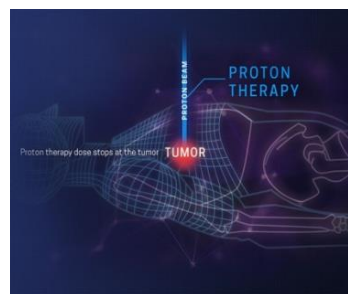
## 1. *Laser driven Compact Ion based Nanotheranostics for Cancer Treatment*

***(Drs Bhuvanesh Ramakrishna and Aravind Kumar Rengan)***

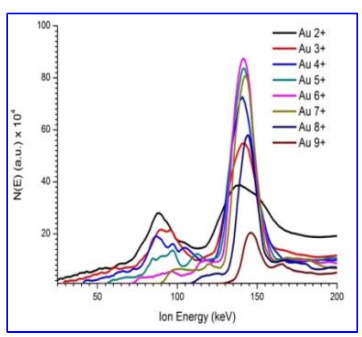
The interaction of intense laser pulses with matter is opening up new frontiers in physics via the production of extreme pressures, temperatures and intense electric and magnetic fields. This is leading to the use of high power laser radiation for exploring the properties of hot dense matter, the production of high-energy particles and radiation and the development of schemes for “table top ion acceleration”. These advances are driven by rapid developments in ultrashort pulse laser technology, which have enabled new regimes in laser power and intensity to be reached. The principal aims of this proposed project are to investigate the usefulness of employing laser driven ion beams for “cancer therapy”. This would provide possibilities of better dose conformity to the treatment target when compared to commonly used photon or electron beams. Proton beams have low entrance dose, sharp penumbra, rapid fall off at the distal edge of the dose distribution, and the maximum rate of energy loss at the end of the range, i.e. the Bragg peak effect. Nanoprobes that act as sensitizers would be deployed to enhance the theranostic effect of the laser driven compact ion therapy.

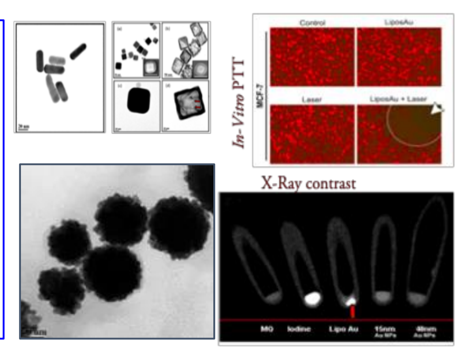





Recent Results: Acceleration of gold ions to 100 KeV from a Table top Laser. Organo-Inorganic hybrid nanosystems (developed in-house) are being explored for theranostics of cancer.

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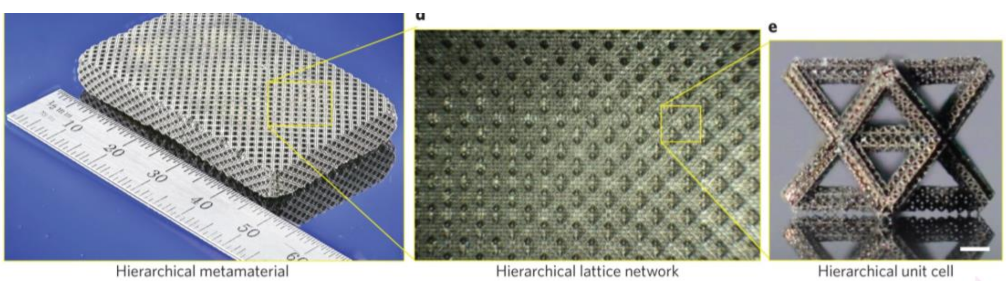
## 2. DAMM: Designing Advanced Mesoscale Metamaterials

(Dr. Prakhar Gupta and Dr. Anurup Datta)

In this project, we will explore the design and fabrication of lightweight mesoscale metamaterials, focusing on their unique properties and potential applications. By manipulating the structure and composition at the mesoscale, novel materials with tailored mechanical properties will be created. Applications span various fields, including aerospace, robotics, biomedical engineering, and telecommunications. Mesoscale metamaterials offer opportunities for lightweight structures with enhanced strength, vibration damping, and electromagnetic shielding capabilities. Through a combination of advanced mathematics, mechanics, design techniques and precise fabrication methods, this research contributes to the development of innovative materials with diverse practical applications. We are looking for students who are having a deep interest in mathematics and mechanics.

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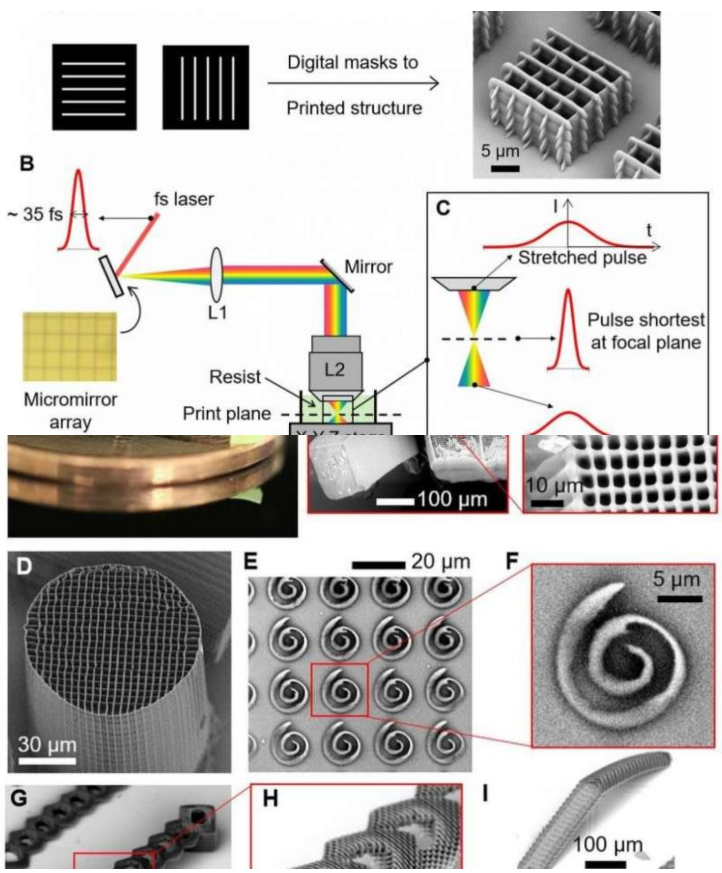
# 3. Femtosecond Laser based Additive manufacturing

**Dr. Anurup Datta and Dr. Bhuvanesh Ramakrishna**

Ultrafast laser-based additive manufacturing, often referred to as ultrafast laser 3D printing or simply ultrafast 3D printing, is an advanced manufacturing technique that utilizes ultrafast lasers to build three-dimensional structures layer by layer. Unlike traditional 3D printing methods that use thermal processes or extrusion techniques, ultrafast laser-based additive manufacturing relies on precise and rapid bursts of laser energy to selectively solidify or ablate material in a layer-by-layer fashion. Ultrafast lasers enable extremely precise control over the material processing, leading to high-resolution prints with intricate details and fine surface finishes. The short pulse durations of ultrafast lasers (typically in the femtosecond range) allow for minimal heat diffusion and reduced thermal damage to the surrounding material, resulting in high-quality prints. Continuous advancements in laser technology, materials science, and process optimization techniques are driving improvements in the speed, efficiency, and cost-effectiveness of ultrafast laser-based additive manufacturing systems. Research efforts are focused on enhancing build rates, reducing material waste, and expanding the range of printable materials. Overall, ultrafast laser-based additive manufacturing holds great promise for revolutionizing manufacturing processes by offering unparalleled precision, speed, and versatility in the fabrication of complex 3D structures across various industries.




*Opt. Express* **2005**, *13*, 4708–4716
*Appl. Phys. A* **2016**, *122*, 1–8

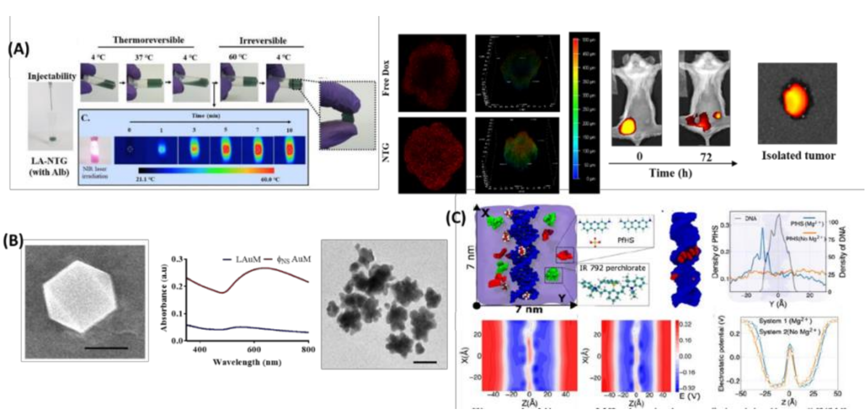
## 4. Physics based multiscale modelling and simulations to decipher the interaction between nanoparticle and cancer cells for efficient therapeutics.

***Dr. Himanshu Joshi (BT) and Dr. Aravind Kumar Rengan (BME)***

Nanotechnology has emerged as an increasingly promising and cost-effective field, particularly in cancer theranostics, attributable to the distinct physico-chemical properties exhibited by nanoparticles compared to their bulk counterparts. Researchers have extensively explored various nanomaterials tailored for targeted and sustained drug delivery, often integrating multiple treatment modalities into a single platform to achieve synergistic effects. Moreover, nanomaterials offer the advantage of selectively accumulating in tumor cells over normal cells, primarily through the enhanced permeation and retention effect facilitated by the compromised lymphatics and vasculature characteristic of cancer cells. Despite the growing interest of in the usage of nanomaterials for cancer theranostics, their full potential in combating tumors is yet to be explored. Theoretical and computational studies could help in rationally designing these nanotherapeutics by understanding the molecular level interaction between the nanomaterial and biological matter in a cellular like environment. Due to the rapid advancement in computer architecture, methods in molecular modeling and machine learning, molecular dynamics (MD) simulation has become a powerful tool to reveal insights into the intricate molecular-level interactions between nanoparticles and cancer cells. These simulations aid in the meticulous design and optimization of nanoparticles for targeted drug delivery to cancer cells, as well as in comprehending the dynamics of cellular interactions, internalization mechanisms, and predicting the toxicological profiles of developed nanosystems.

The principal aim of this proposed project is to develop a robust computational framework to understand the interaction of nanomaterials with proteins and lipid assemblies using multiscale modeling approaches. We plan to build on *ab-initio* DFT calculations, QM/MM, all-atom and coarse-grain MD simulations, and continuum Navier–Stokes equations. The machine learning-based force-fields potentials will be integrated to improve the accuracy of all-atom MD simulations. Information deduced from simulation trajectories and analysis will be used to understand the binding mechanisms which is expected to help in rationally designing experiments, understanding the experimental outcome, and prospective clinical trials.

Recent Results: (A) Lipo-polymeric hydrogel, (B) Gold coated phage nanosomes being developed are explored for cancer theranostic applications (C) MD simulation depicting interaction of intercalating dye and drug to DNA based nanomatrix

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