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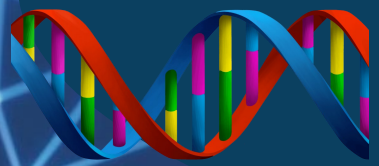
Data-Driven Inverse Design of Low-Dimensional Nanocarbons: Revealing Hidden Growth-Properties Relationships and Identifying Universal Descriptors



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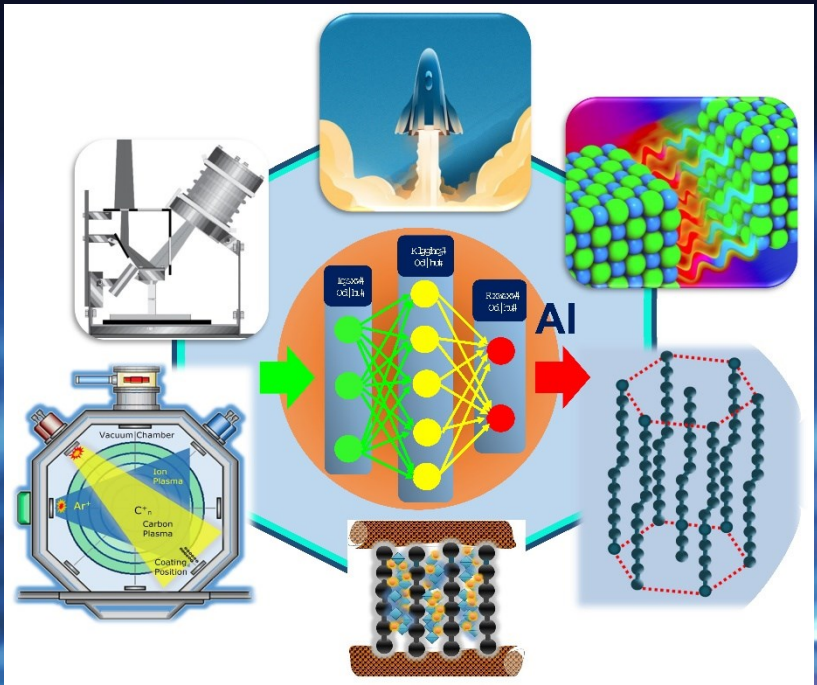
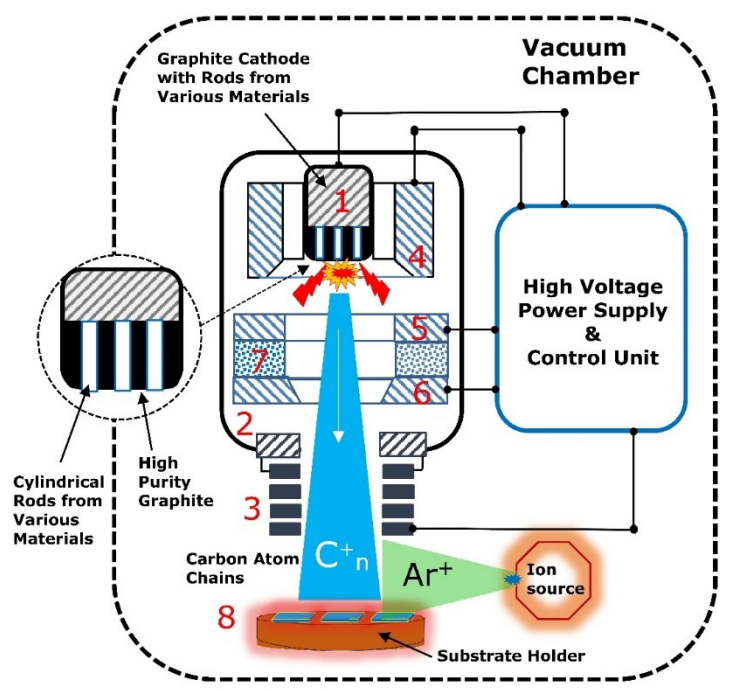


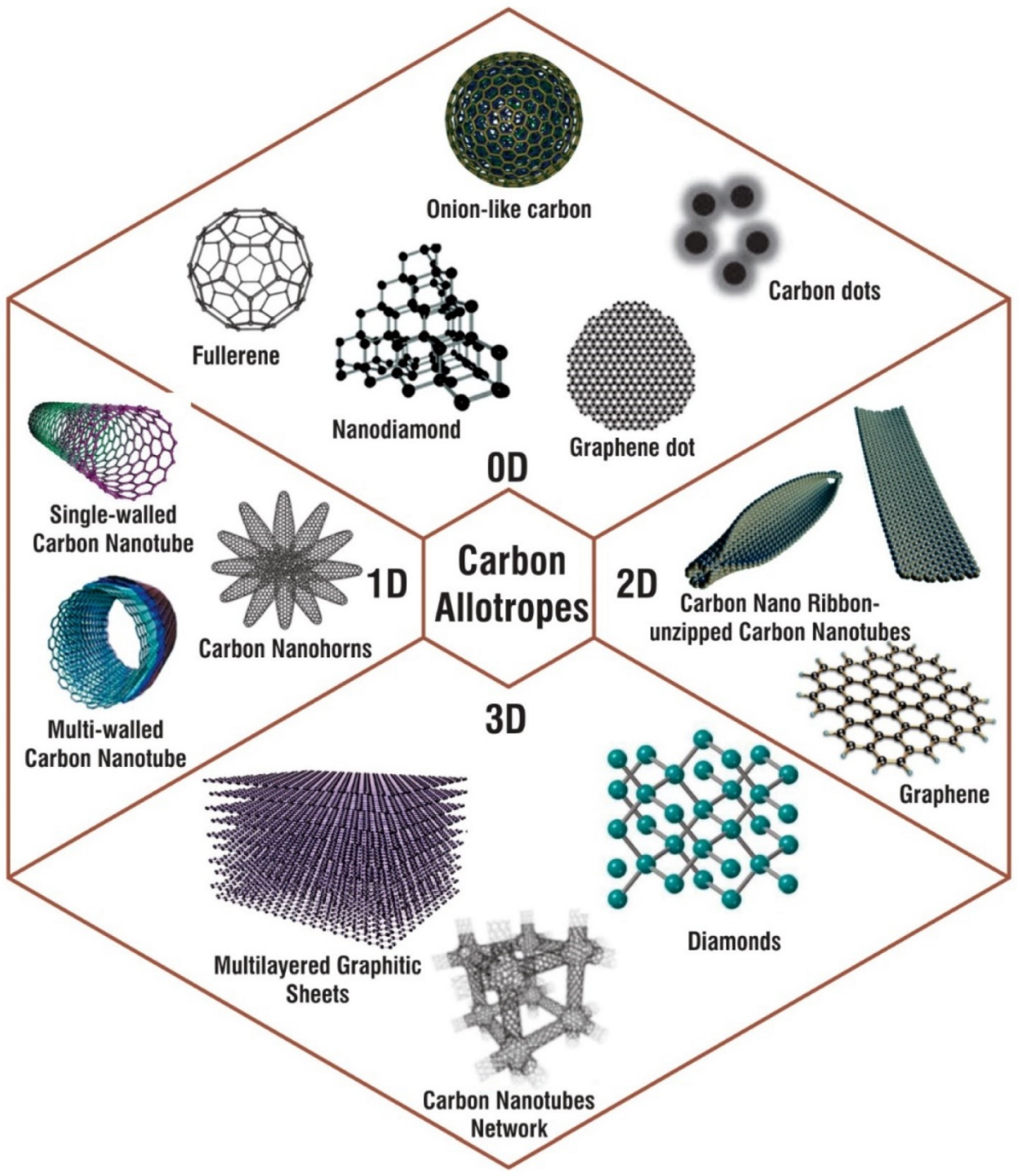


THE OBJECTIVE OF PRESENTATION

Our research aims to develop an innovative and targeted data-driven inverse design strategy, which is built upon the carbon nanomaterial genome approach. The primary objective of this strategy is to unlock the latent potential of nanocarbons and revolutionize the field.

By adopting our proposed strategy, we anticipate a significant transformation in our ability to design low-dimensional nanocarbons in an inverse manner. Through gaining critical insights into the synthesis process, we can fine-tune and control the parameters to achieve desired attributes in the resulting nanocarbons.

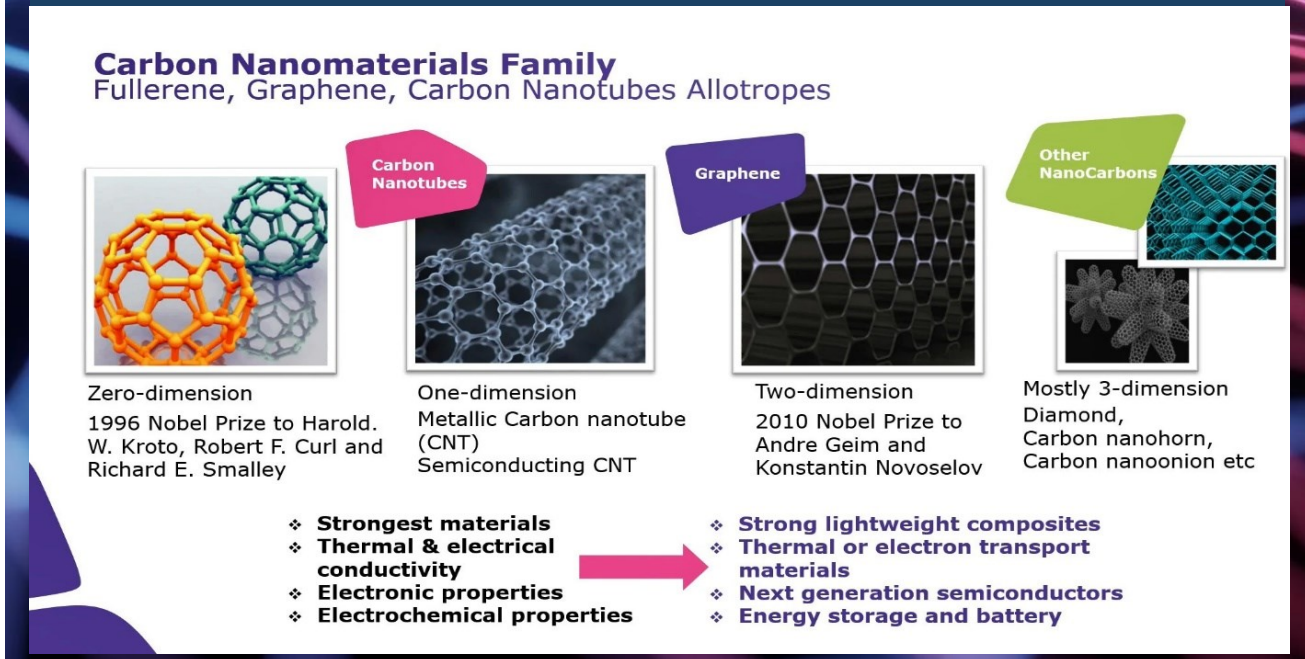
This approach enables us to accelerate the discovery and design of nanocarbons with tailored properties, saving time and resources compared to traditional trial-and-error-based methods.

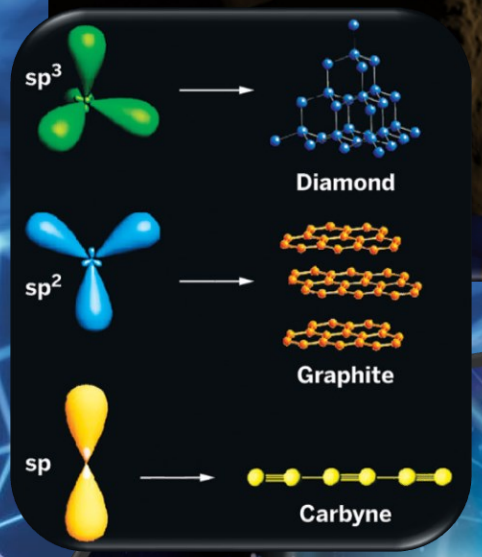


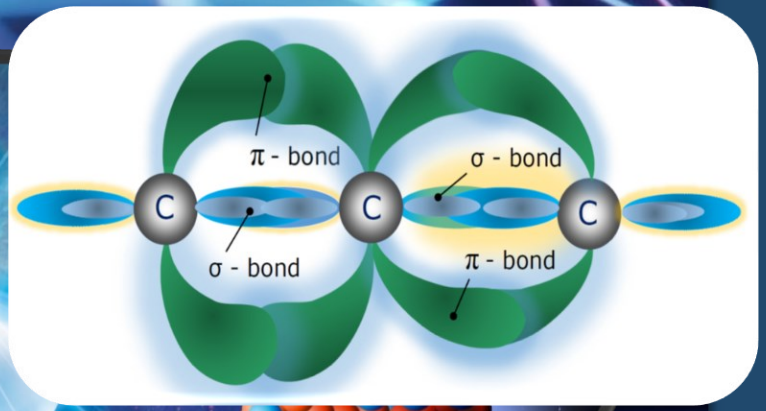
The transformative potential of unlocking the latent capabilities of low-dimensional nanocarbons

Recent advancements in nanomaterials science have been catalyzed by low-dimensional nanocarbon allotropes, especially the extraordinary potential of carbyne. This true one-dimensional carbon chain promises unrivaled possibilities as the fundamental building block for engineering the next generation of tailored nanocarbons.

Low-dimensional carbon-based nanomaterials serve as highly adaptable and robust building blocks that can revolutionize diverse practical applications. They offer immense potential for engineering advanced materials with tailored properties and functionalities.







Carbyne, an allotropic form of carbon, represents a fascinating example of the many unknowns that still exist in the realm of science.

Unlike most carbon structures found on Earth, carbyne does not naturally exist under terrestrial conditions. Instead, it is thought to be formed in the unique environments of outer space.

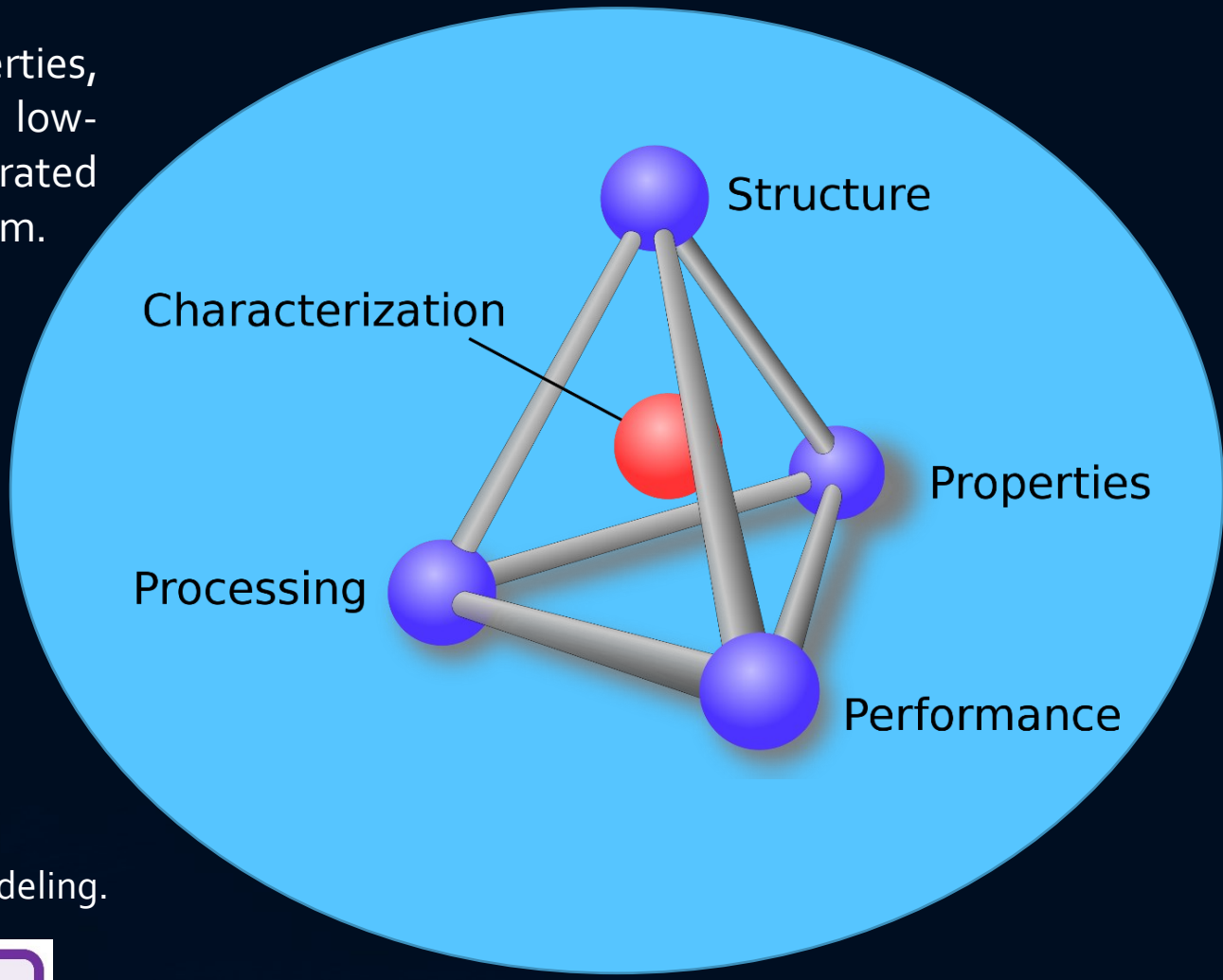
The formation of cosmic carbyne crystals is hypothesized to occur through various mechanisms, one of which involves the intense synchrotron radiation experienced under a coronal photon flux in the interplanetary medium.

The existence of cosmic carbyne provides valuable insights into its formation mechanisms and the environments it encounters.

By investigating carbyne and its formation process, we expand our understanding of carbon's behavior in extreme conditions and the potential applications of such unique structures.

The Materials Science Tetrahedron Paradigm

The connections between the structure, properties, performance, processing, and characterization of low-dimensional nanocarbons are effectively demonstrated through the Materials Science Tetrahedron (MST) paradigm.



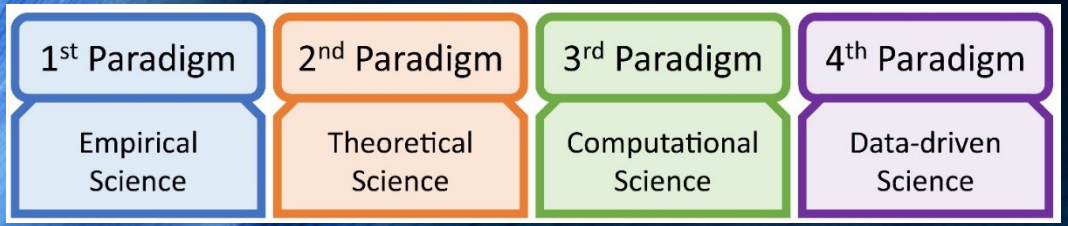
The four paradigms of science and its application toward predictive modeling.

1st Paradigm	2nd Paradigm	3rd Paradigm	4th Paradigm
Empirical Science	Theoretical Science	Computational Science	Data-driven Science

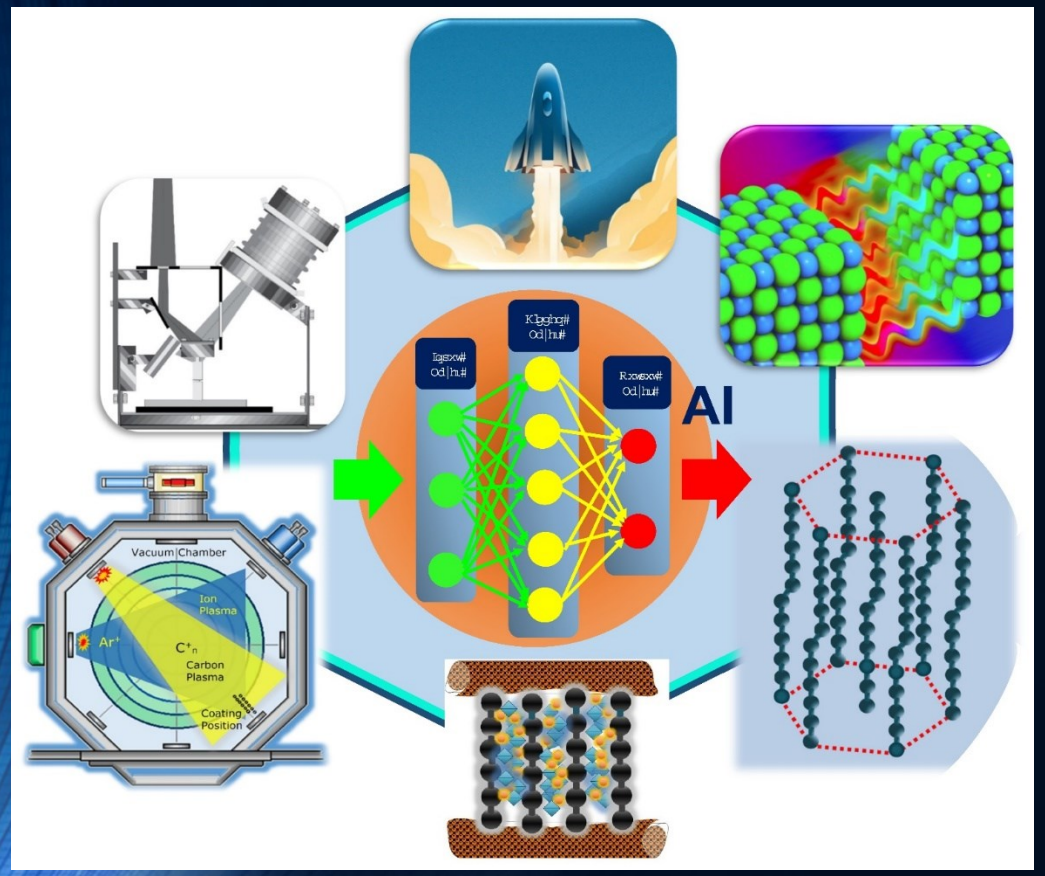
AI in Materials Science:
A Catalyst for Breakthroughs in Material Technologies

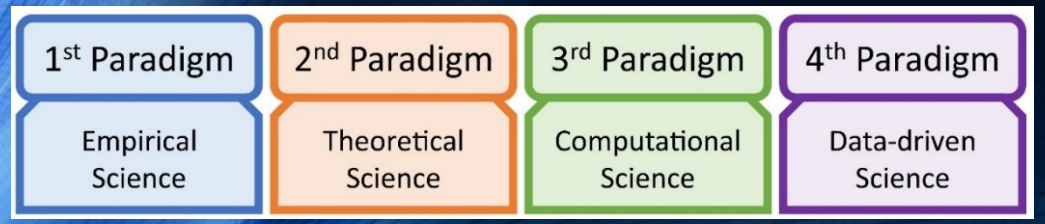
Artificial Intelligence (AI) is revolutionizing numerous industries, and materials science is no exception. As a catalyst for breakthroughs in material technologies, AI is poised to transform the field, accelerating innovations and pushing the boundaries of what is possible.

The advent of AI in nanomaterials science is a game-changer, offering the potential to significantly speed up the development of new nanomaterials.
Traditionally, the discovery and development of new nanomaterials have been a time-consuming and costly process, often taking several years or even decades. However, with the application of AI, this process can be expedited. Machine learning algorithms can analyze vast amounts of data to predict the properties of new nanomaterials, significantly reducing the time and cost involved in their development.



The Integration of the Materials Science Tetrahedron Paradigm with Deep Nanomaterials Informatics

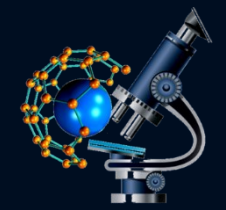




The integration of the Materials Science Tetrahedron paradigm with deep nanomaterials informatics offers a synergistic approach toward advancing the field of nanomaterials science.

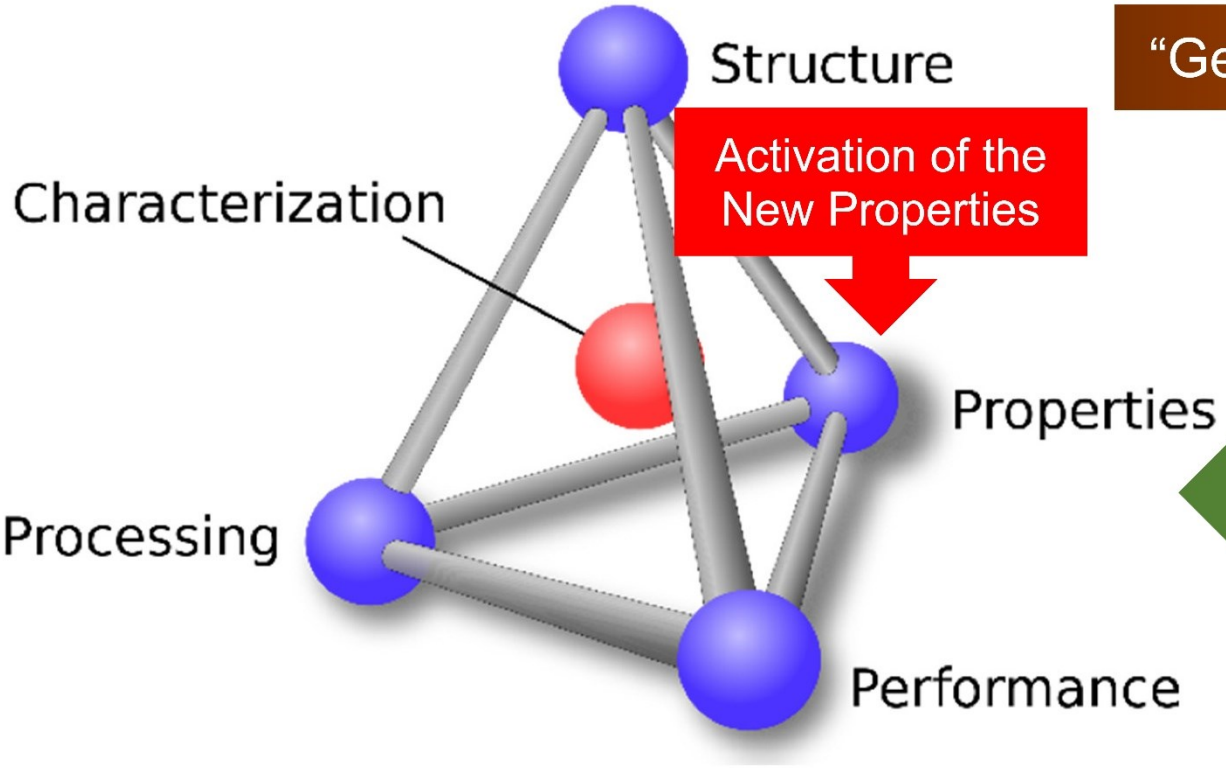
This integration enables researchers to leverage the power of both frameworks, accelerating nanomaterials discovery, optimization, and design, ultimately leading to transformative advancements in nanotechnology.

The need for the development of a Digital Twin of the Materials Science Tetrahedron Paradigm arises from the desire for a comprehensive understanding of carbon nanomaterials, unraveling their complexities, leveraging data and machine learning, enabling predictive modeling and inverse design, and ultimately accelerating innovation and applications in various industries.



Integrating Materials Science Tetrahedron (MST) Paradigm with Deep Nanomaterials Informatics: A Data-Driven Nano-Carbon Genome Approach

Materials Science Tetrahedron Paradigm



Digital Twin: Data-Driven Nano-Carbon Genome Approach

"Genetic Code" Modification

Experimental Data

Feedback Data

Phonon Engineering and Manipulation at Nanoscale

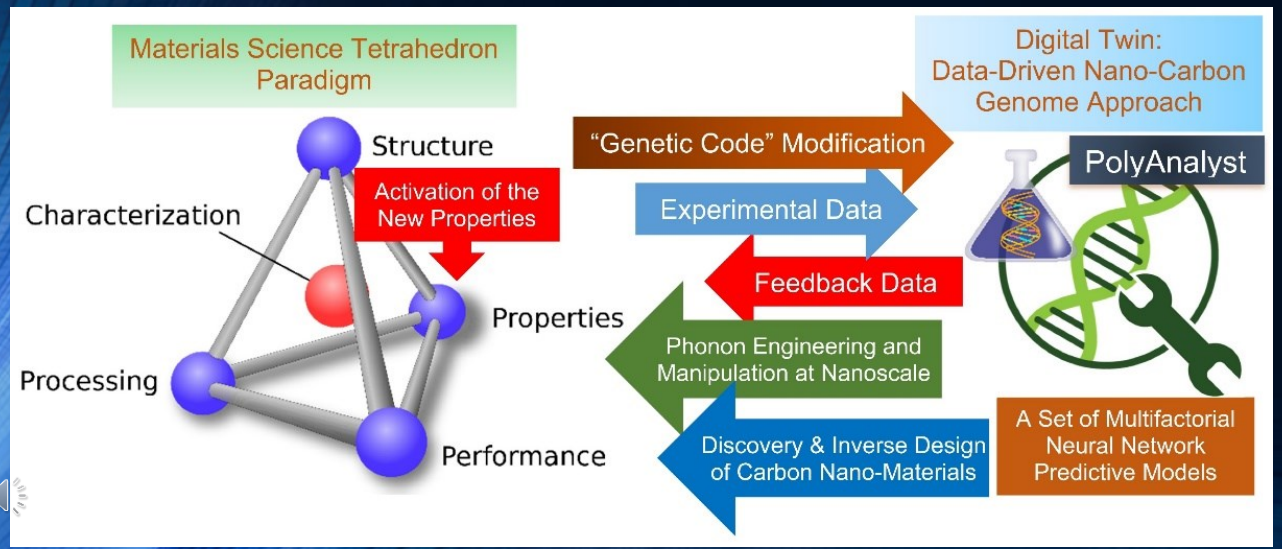
Discovery & Inverse Design of Carbon Nano-Materials

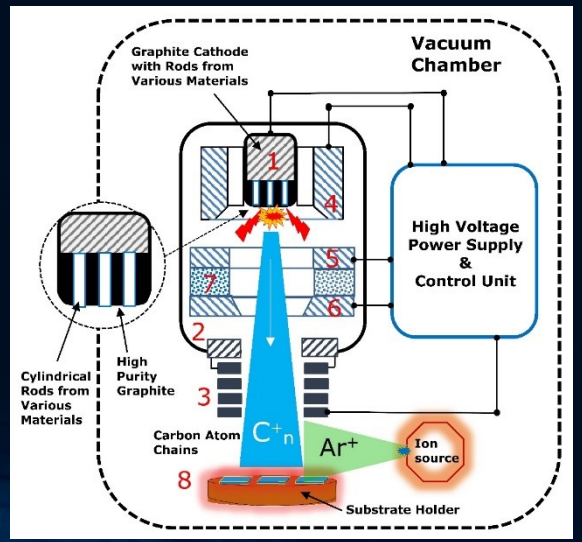
PolyAnalyst

A Set of Multifactorial Neural Network Predictive Models

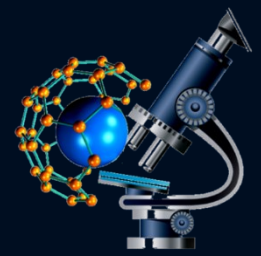
Unleashing the Power of Data:
Data-Driven Carbon Nanomaterials Genome Approach

The nanocarbon genome isn't a physical genome as we understand it in biology.
It doesn't contain the DNA of living organisms.
Instead, it's a conceptual framework, a way of understanding and categorizing the vast diversity of nanocarbon materials.
Imagine a vast library filled with every possible variation of nanocarbon, each with its unique properties and potential applications. That's the nanocarbon genome.
At its core, this genome is data-driven. It's built on the collection, analysis, and interpretation of vast amounts of information about the structures and properties of nanocarbon materials.
With every new piece of data, the genome grows, expanding our understanding of what nanocarbon is capable of.





The Data-Driven Nanocarbon Genome is Not Just a Concept; It is a Roadmap to the Future



The Data-Driven Carbon Nanomaterials Genome Approach is a methodology that combines data-driven techniques, machine learning, and materials science to gain insights into the behavior and properties of carbon nanomaterials.

This approach aims to create a comprehensive understanding of these materials by effectively leveraging the vast amount of available data.
The key steps of the data-driven carbon nanomaterials genome approach are as follows:
1. Data Collection and Curation.
2. Data Analysis and Feature Engineering.
3. Machine Learning Model Development.
4. Predictive Modeling and Inverse Design:
The trained machine learning models are then used for predictive modeling and inverse design. Researchers can input desired properties or characteristics of nanomaterials into the models to obtain the optimal synthesis parameters that would result in the desired outcome. This enables targeted and efficient design of nanomaterials with specific properties.
5. Experimental Validation and Iteration: The predicted synthesis parameters are then experimentally validated to confirm their accuracy and effectiveness.

The data-driven carbon nanomaterials genome approach allows researchers to uncover hidden relationships and understand the complexities of carbon nanomaterials.

Outline of the Machine Learning Workflow for Developing Multifactorial Predictive Models of Carbon Nanomaterials Grown using A Data-Driven Genome Approach

Set of Multifactorial Neural Network Predictive Models: Employing state-of-the-art neural network architectures, we develop a set of Multifactorial Neural Network Predictive Models. These models effectively capture the complex multifactorial relationships between synthesis conditions and nanomaterial properties, enabling accurate predictions and insights.

Experimental Data Collection and Computational Data Generation

Raw Data Preprocessing - Data Cleaning

Data Test Set

Data Training Set

Data Validation Set

Selection of Algorithms

Key Descriptors Identification

Construction of the Multifactorial Neural Network Predictive Models

Model Training

Model Evaluation & Validation

Model Optimization

The Activation of the Carbon Nanomaterials "Genetic Code"

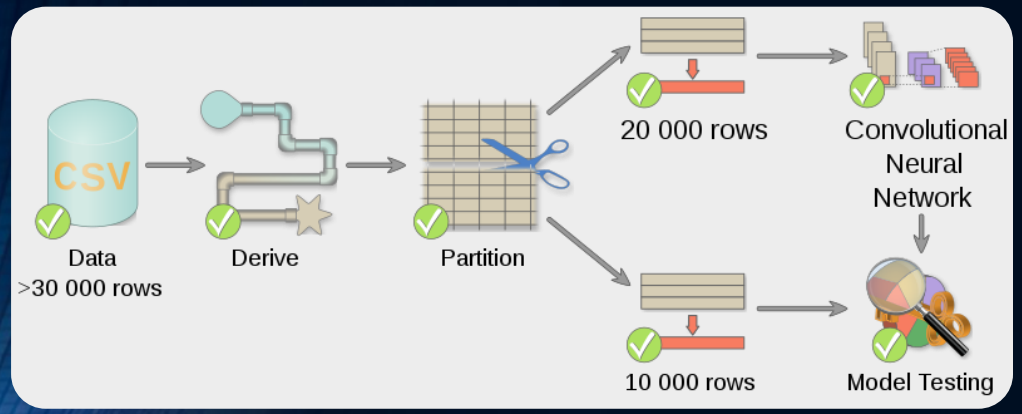
Predictive Modeling & Inverse Design

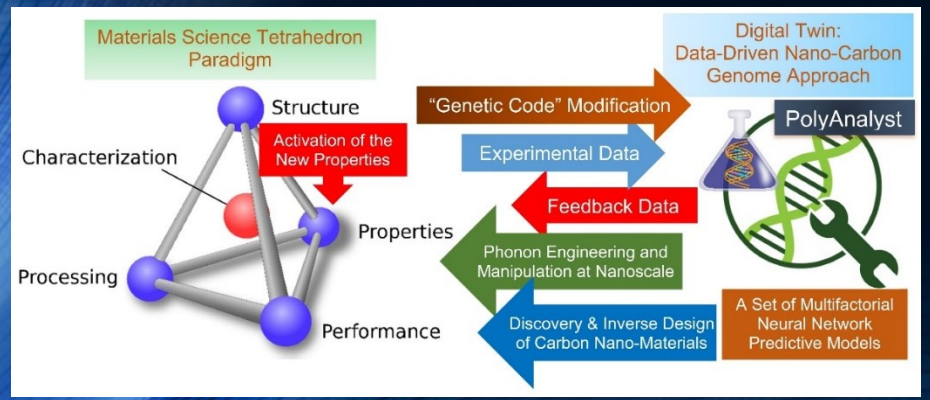
Model Deployment

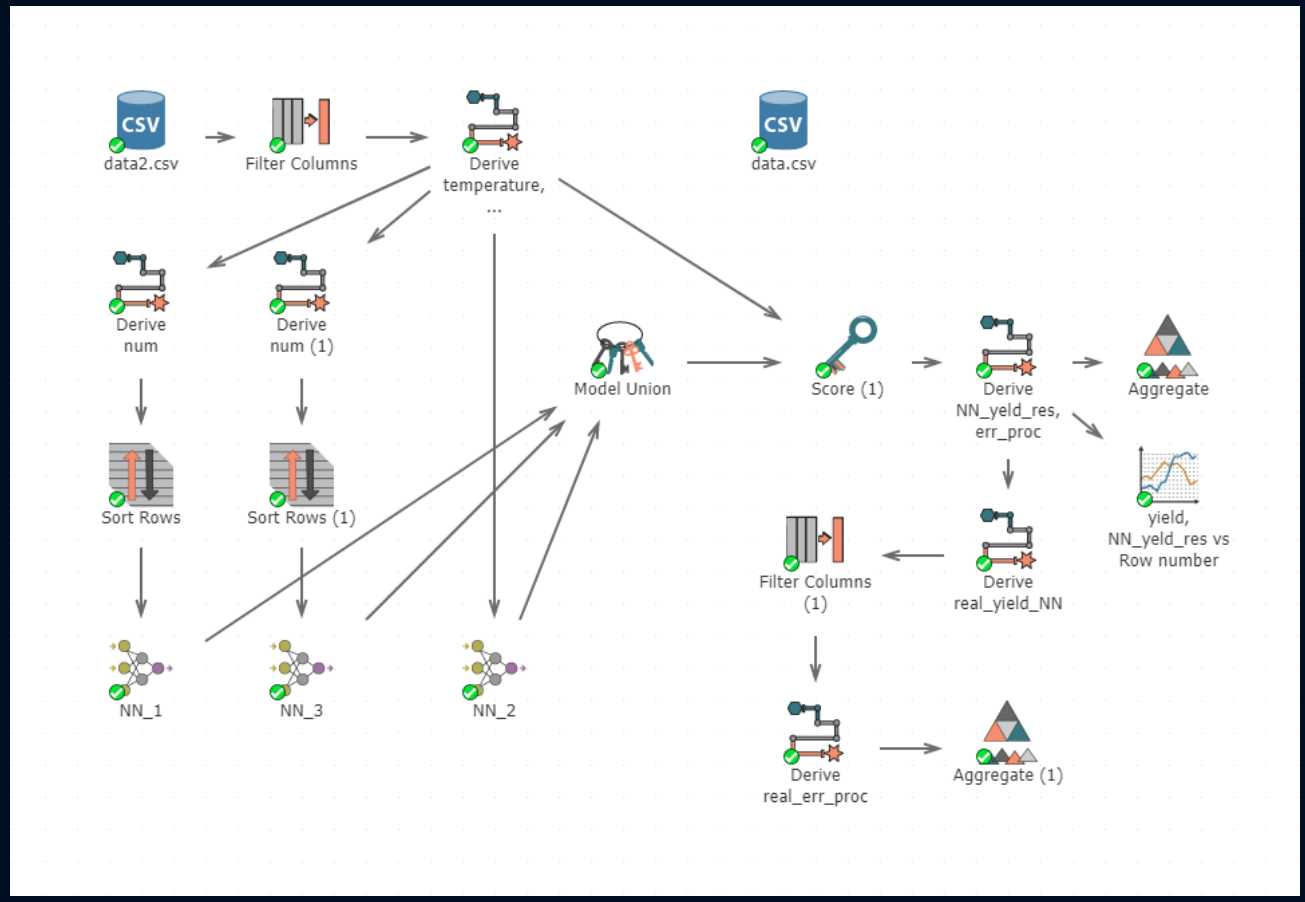
Model Continuous Improvement

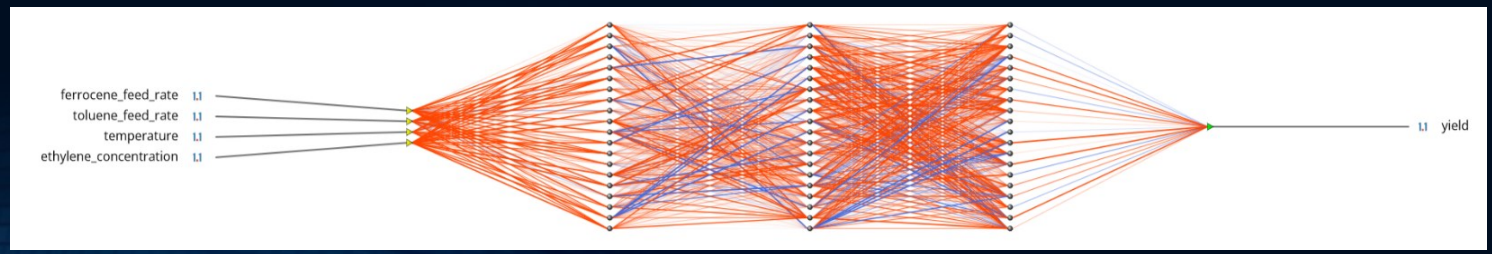
Development of the Multi-Factor Neural Network Predictive Models Using PolyAnalyst Analytical Platform

For the development of the multi-factor neural network predictive models we use the Analytical Platform PolyAnalyst – https://www.megaputer.com/polyanalyst/

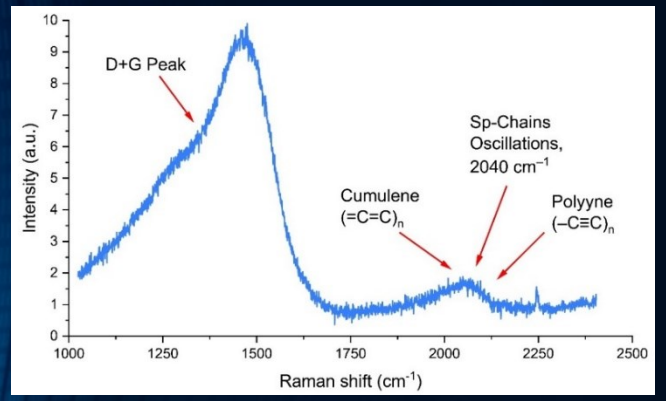


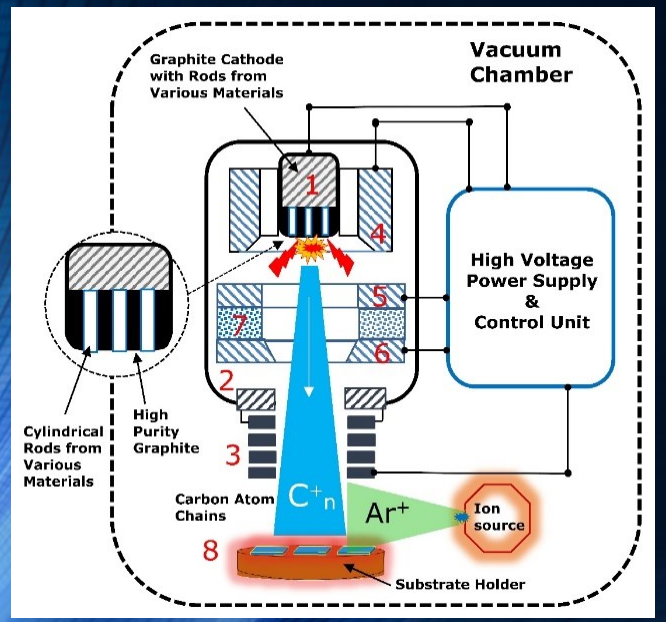






Identification of Universal Descriptors for Carbon Nanomaterial Properties



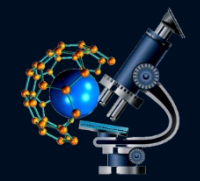


Universal descriptors play a crucial role in guiding inverse design and optimizing the synthesis parameters to achieve desired properties in carbon nanomaterials.

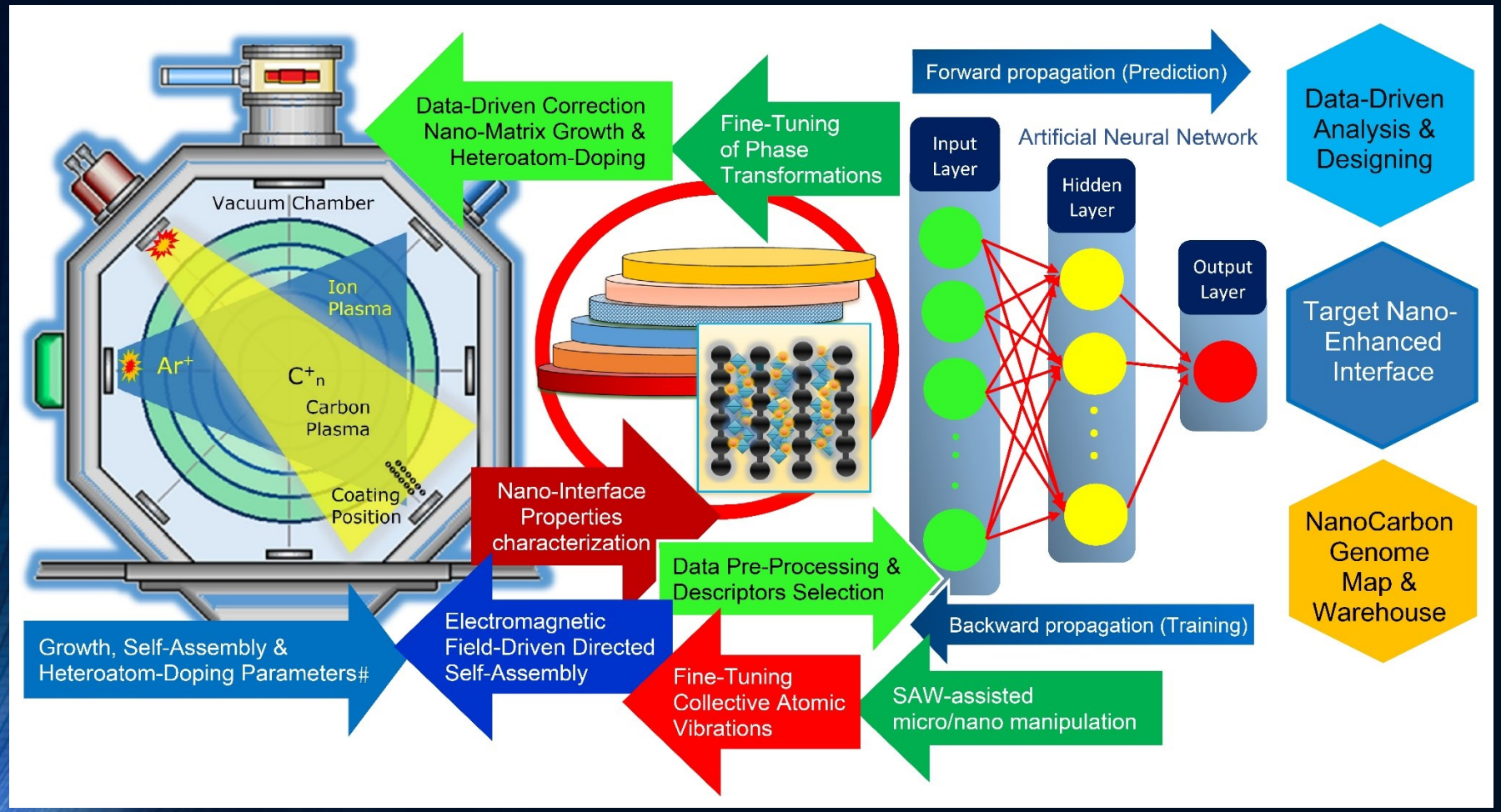
Universal descriptors are essentially key parameters or characteristics that have a significant impact on the properties of nanomaterials, regardless of their specific structure or synthesis method. By identifying these universal descriptors, we can streamline the design process and make it more efficient.

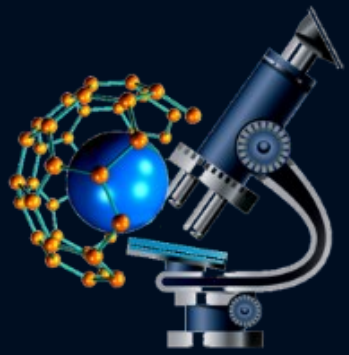
By analyzing the relationships between growth parameters and resulting properties, we can uncover hidden growth-properties relationships and identify universal descriptors.

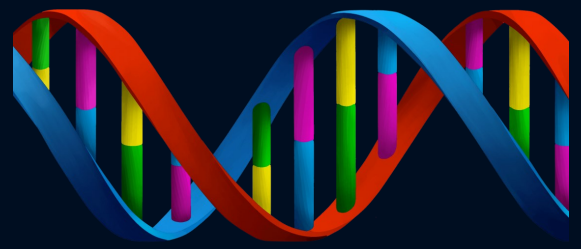
The identification of universal descriptors involves in-depth analysis and data mining techniques applied to the collected and curated data on carbon nanomaterials. Through advancements in machine learning algorithms and statistical analysis, we can reveal hidden relationships between growth parameters and resulting properties.
Using these techniques, we can extract insights from the data and identify the critical factors that impact the properties of the nanomaterials.
Once universal descriptors are identified, they serve as guidelines for the inverse design of carbon nanomaterials, allowing us to optimize the growth conditions to achieve desired properties in the nanocarbons.



Identification of Universal Descriptors for Carbon Nanomaterial Properties







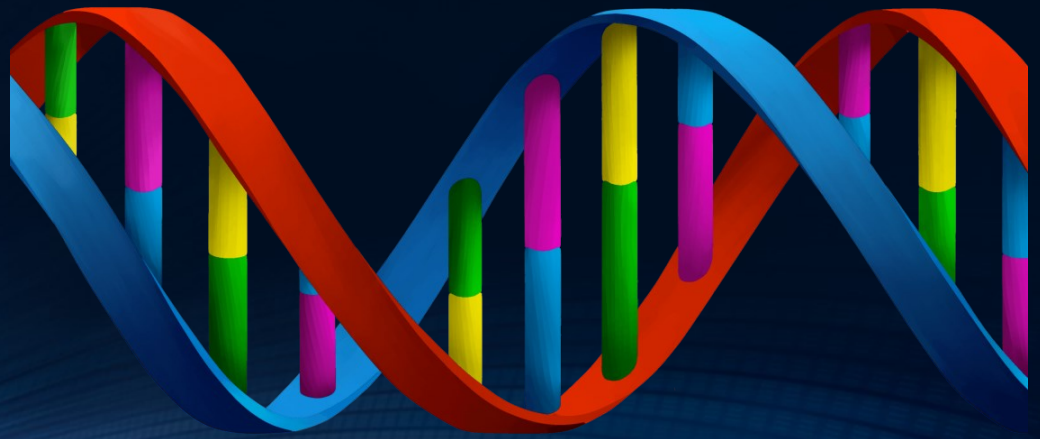
Schematic illustration of the data-driven inverse design methodology used to precisely tune and optimize the properties of low-dimensional nanocarbons. The approach integrates theoretical modeling, precision synthesis, characterization, and machine learning to enable predictive engineering of low-dimensional nanocarbons.

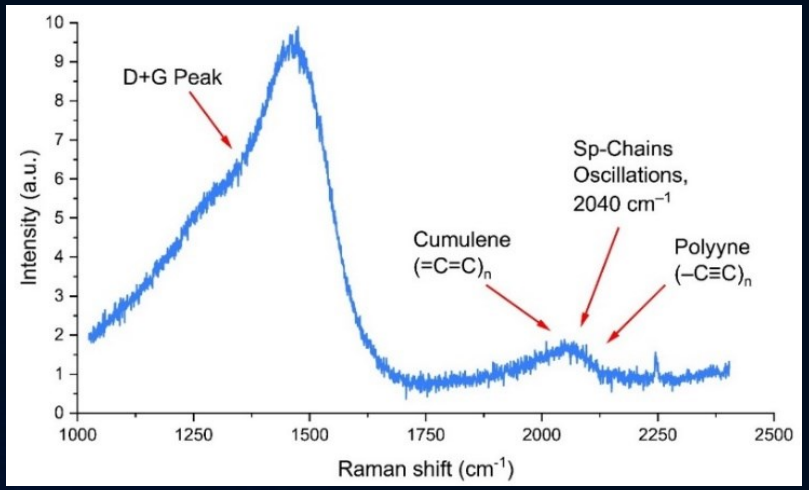
The “Genetic Code” in the Data-Driven Carbon Nanomaterials Genome Approach

In the data-driven carbon nanomaterials genome approach, each carbon nanomaterial possesses a unique signature or "genetic code". This genetic code represents the interconnected set of distinct properties and characteristics that define the nanomaterial.

This conditional concept represents the underlying relationships between various factors, such as structure, composition, size, and processing conditions, and how they influence the physical properties of the nanomaterials. By analyzing this "genetic code," researchers can uncover valuable insights into how specific combinations of these factors determine the unique characteristics of carbon nanomaterials.

By decoding this genetic code, we can engineer nanomaterials with desired properties, predict and manipulate the properties of carbon nanomaterials to suit specific applications.



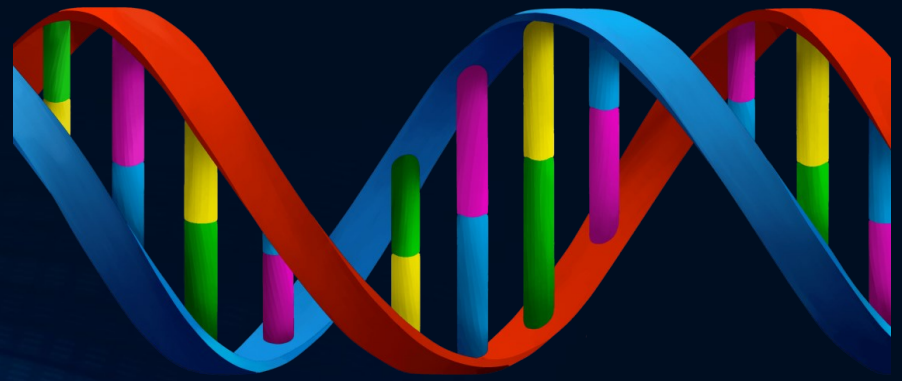


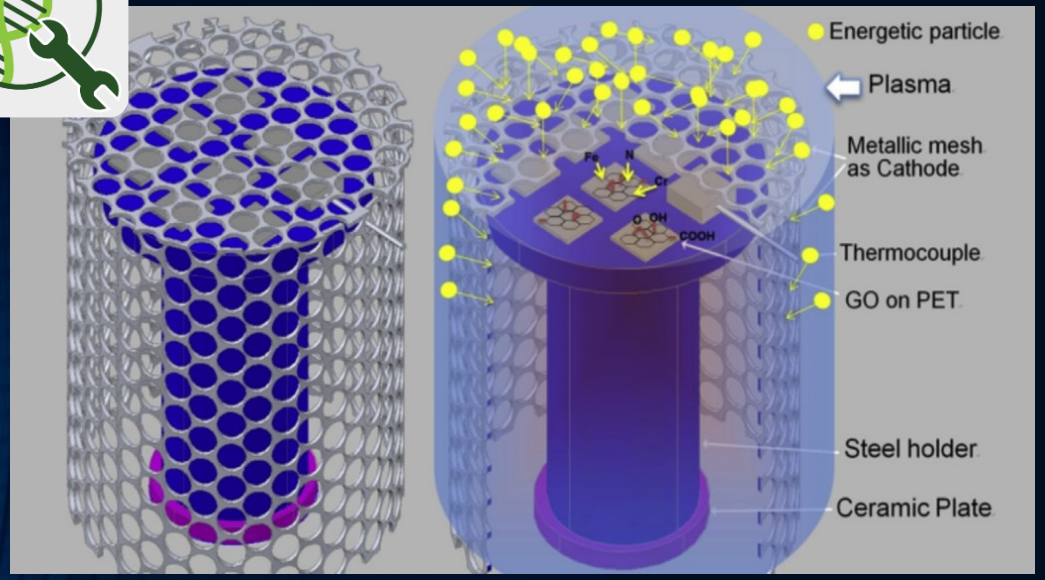
Activating the Carbon Nanomaterials' "Genetic Code": Unleashing New Neural Connections

By actively exploring and creating new neural connections within the Carbon Nanomaterials "Genetic Code" framework, we can unravel the complex relationships between synthesis parameters, nanocarbon structures, and resulting properties.

This understanding is crucial for tailoring the synthesis process to achieve desired structural characteristics and, subsequently, the desired properties of the low-dimensional nanocarbons.

Creating new neural connections within the Carbon Nanomaterials "Genetic Code" allows researchers to elucidate the synthesis-structure-property relationships in low-dimensional nanocarbons.
By actively exploring and establishing these connections, researchers can uncover the hidden knowledge necessary to tailor the synthesis process and achieve desired properties in carbon nanostructures.





ASP technology provides an effective approach for controllable and uniform heteroatom doping of low-dimensional nanocarbons while preserving their nanostructure, composition, and properties.

ASP allows introduction of heteroatoms like nitrogen, boron, sulfur into the lattice of nanocarbons by using different gas compositions.

Active Screen Plasma (ASP) surface engineering for functionalizing low-dimensional nanocarbons:

Active screen plasma (ASP) is a low-temperature and low-pressure plasma technology of surface engineering, which was developed at the University of Birmingham in the early 2000s .
Remote plasma nature avoids damage or degradation of nanocarbon structures.

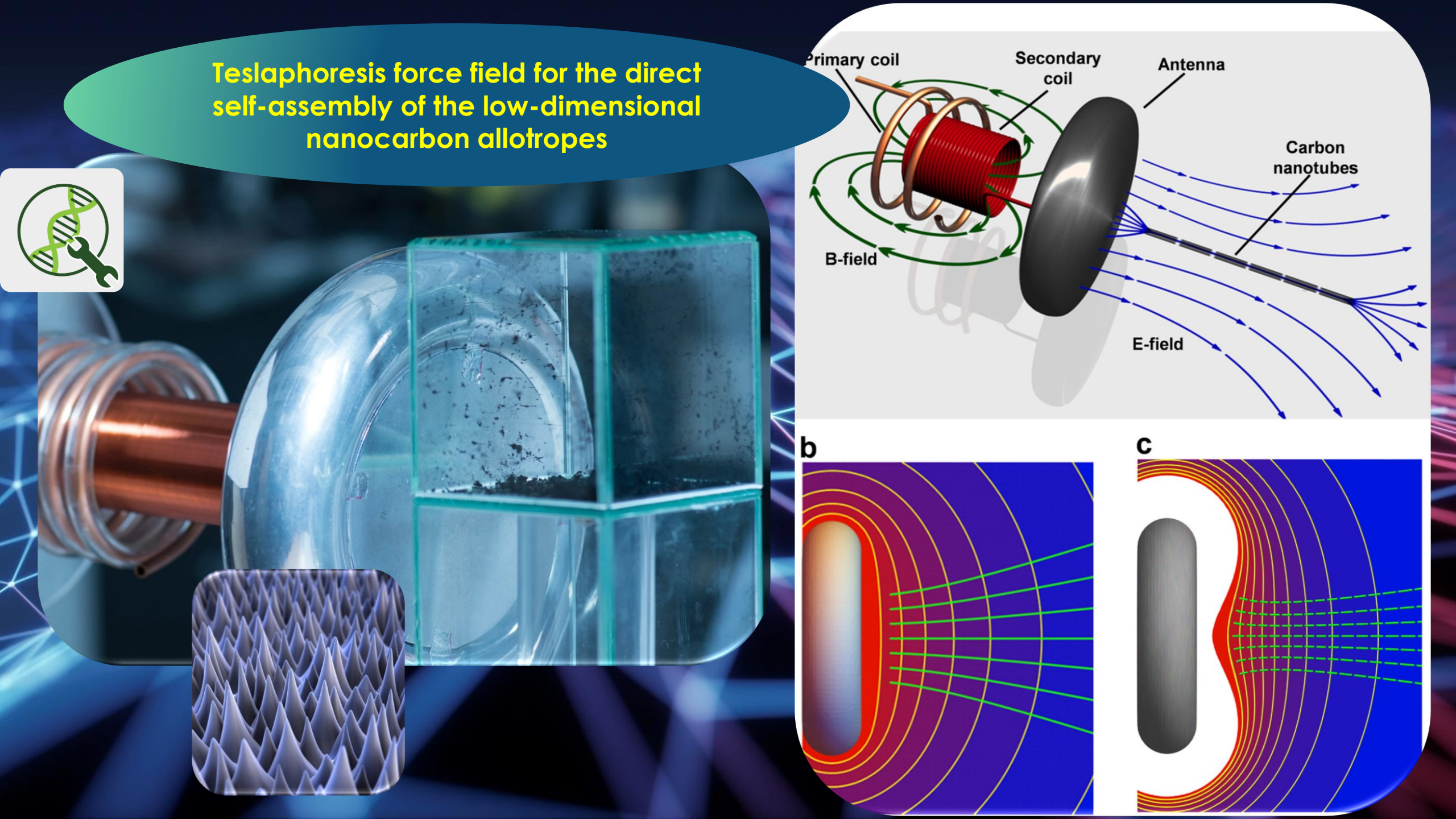
The active screen is a metallic mesh that surrounds the sample and serves as the cathode. The chamber walls serve as the anode.

Plasma discharge takes place on the active screen surface rather than directly on the sample surface. This allows for more control over the plasma-sample interactions.

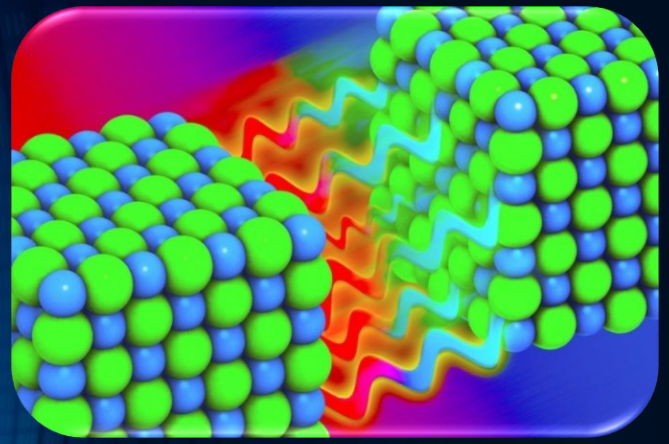
Can simultaneously reduce, dope, and deposit nanoparticles on nanocarbons in a single step process.

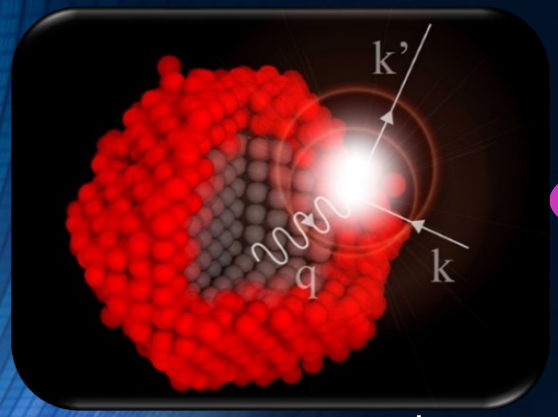
Enables deposition of metallic nanoparticles like Ag, Ni, Pt on nanocarbons to enhance electrical, electrochemical, catalytic properties.

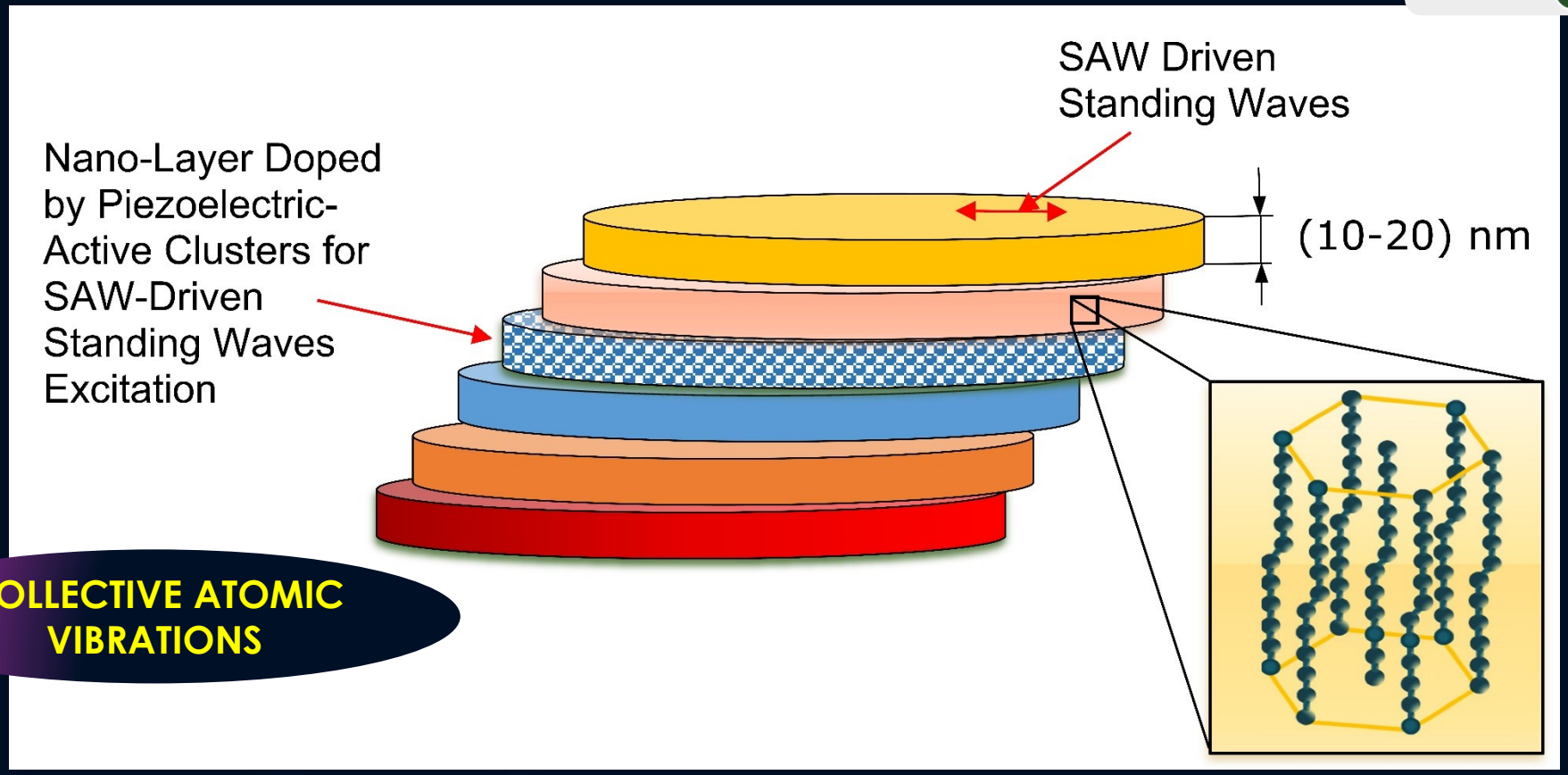
Teslaphoresis force field for the direct self-assembly of the low-dimensional nanocarbon allotropes



Phonon Engineering Through the Use of Multilayer Nano-Interfaces: Programmable excitation of the collective atomic vibrations self-synchronization.





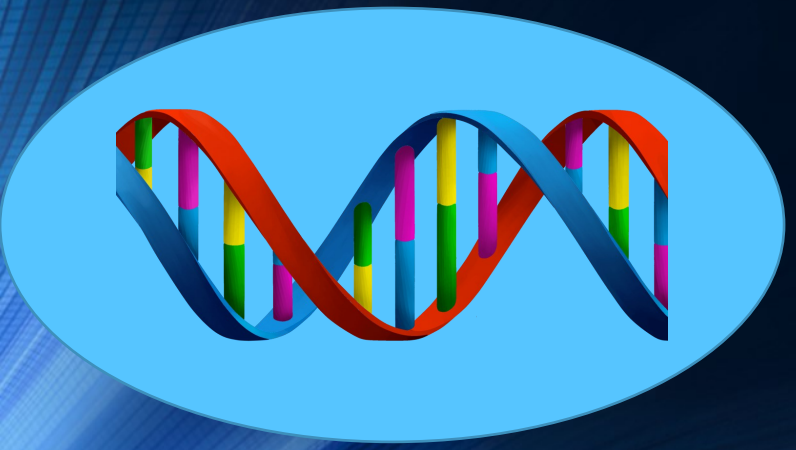


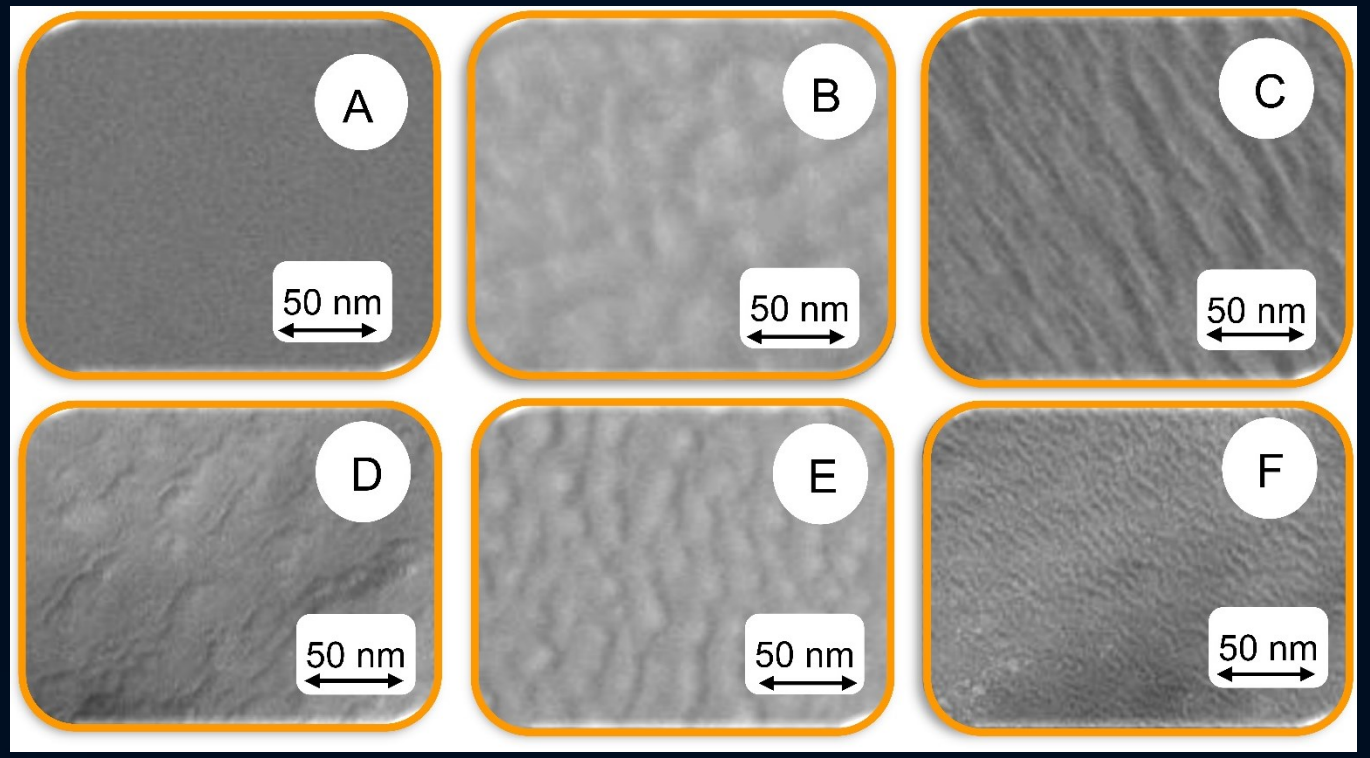
COLLECTIVE ATOMIC VIBRATIONS

Phonon engineering involves tailoring the properties and behavior of phonons in materials to achieve desired functionalities. By leveraging multilayer nano-interfaces, we can precisely control phonon transport, scattering, and energy conversion processes. The use of multilayer nano-interfaces allows for programmable excitation of collective atomic vibrations. By leveraging phonon engineering, we can unlock new functionalities and optimize the behavior of materials for specific applications.

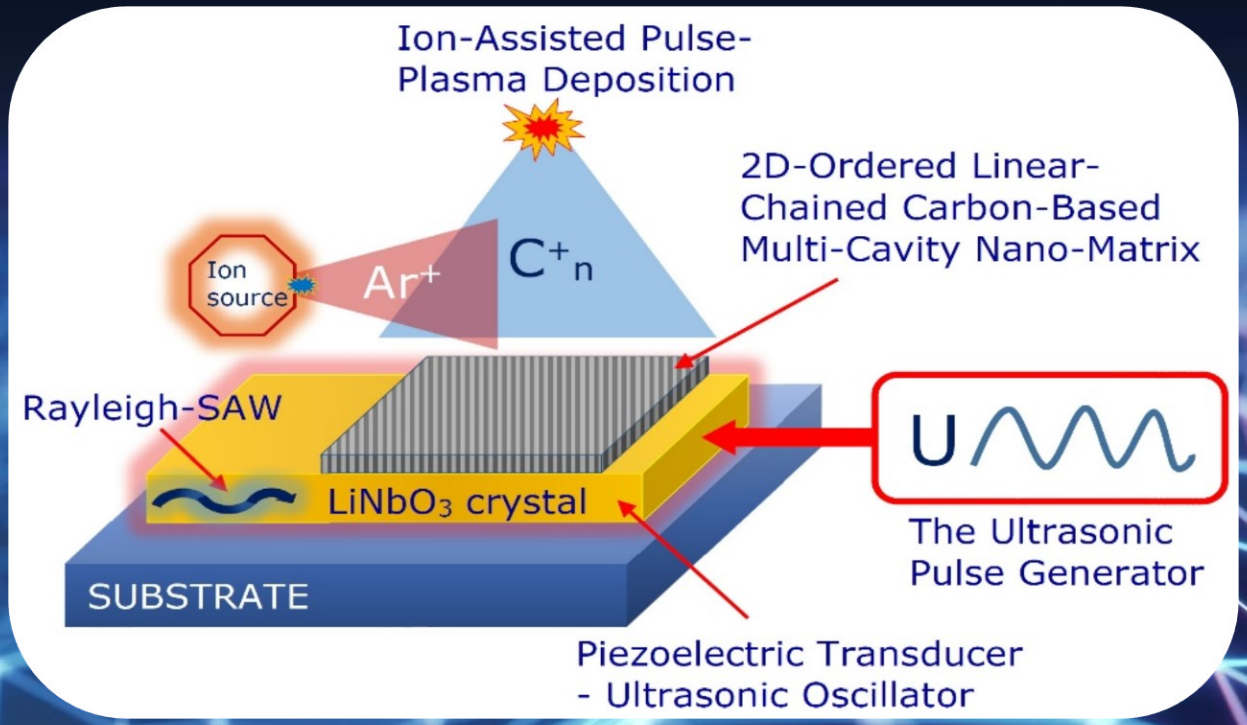
MODIFYING THE "GENETIC CODE" OF A SPECIFIC PHYSICAL PROPERTY IN CARBON NANOMATERIALS

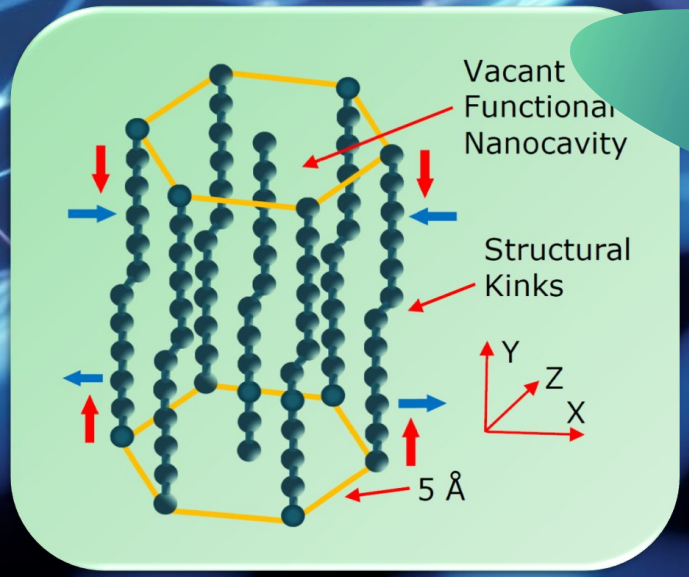
One example of modifying the "genetic code" of a specific physical property in carbon nanomaterials is achieved through the creation of novel nano-oscillatory systems. These systems involve the formation of oriented nano-patterns, which facilitate the surface acoustic wave-driven excitation of phonon wave resonance. This, in turn, enables us to programmatically control and manipulate the properties of the nanomaterial.





The examples of the self-organized patterns of excitation for the amorphous carbon nitride (a-C:N) film samples grown at various ion assistance energies.
The transmission electron microscopy has shown that the structure of the sample deposited without ion assistance is homogeneous, while the structure of ion-assisted samples is heterogeneous. The specific conductivity of ion-assisted samples is (103–104) times larger than the conductivity of the samples deposited without ion assistance. Similar patterns corresponding to ripple-like surface structure were observed for amorphous carbon films irradiated with off-normal ion beam during their formation or after deposition.



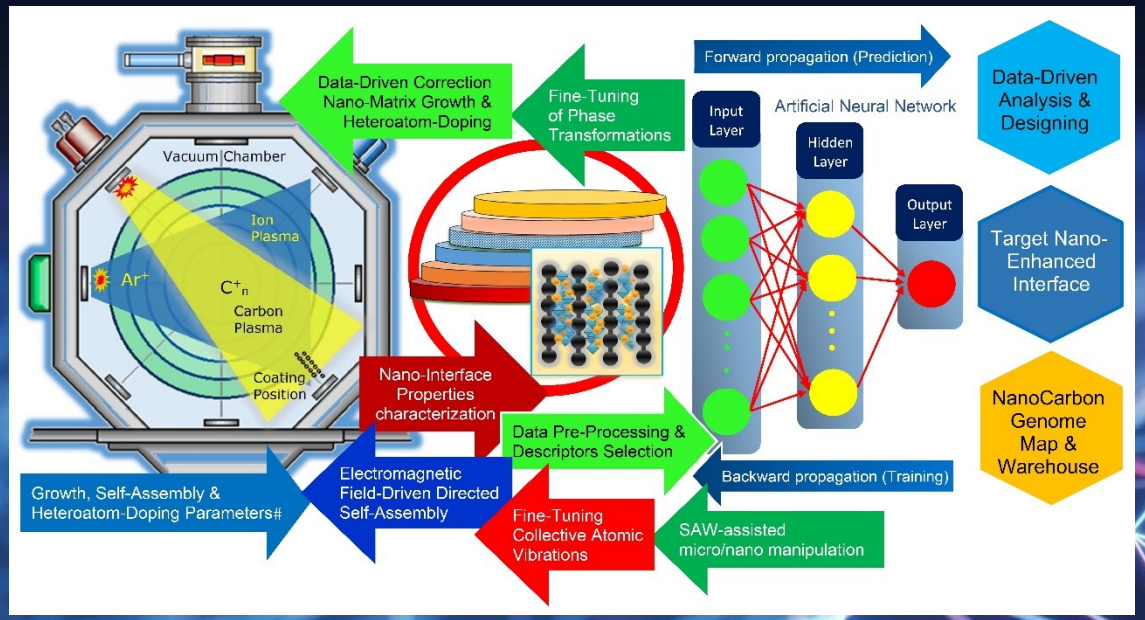


Modifying the Raman Response

The piezoelectric surface acoustic waves can induce atomic-level changes to the growing nanocarbon thin film, modifying its phonon properties and vibrational characteristics, which are then detectable through shifts and variations in the Raman spectroscopic response.

Surface acoustic waves are high-frequency mechanical vibrations that propagate along the surface of a material.
They are typically generated by applying an oscillating electric signal to a piezoelectric substrate.
When a surface acoustic wave travels through a growing nanocarbon film, it interacts with the carbon atoms in the lattice structure of the film.

This interaction causes the atoms to vibrate and oscillate with the frequency of the surface wave.
In essence, the acoustic wave transfers some of its vibrational energy to the atoms in the film.



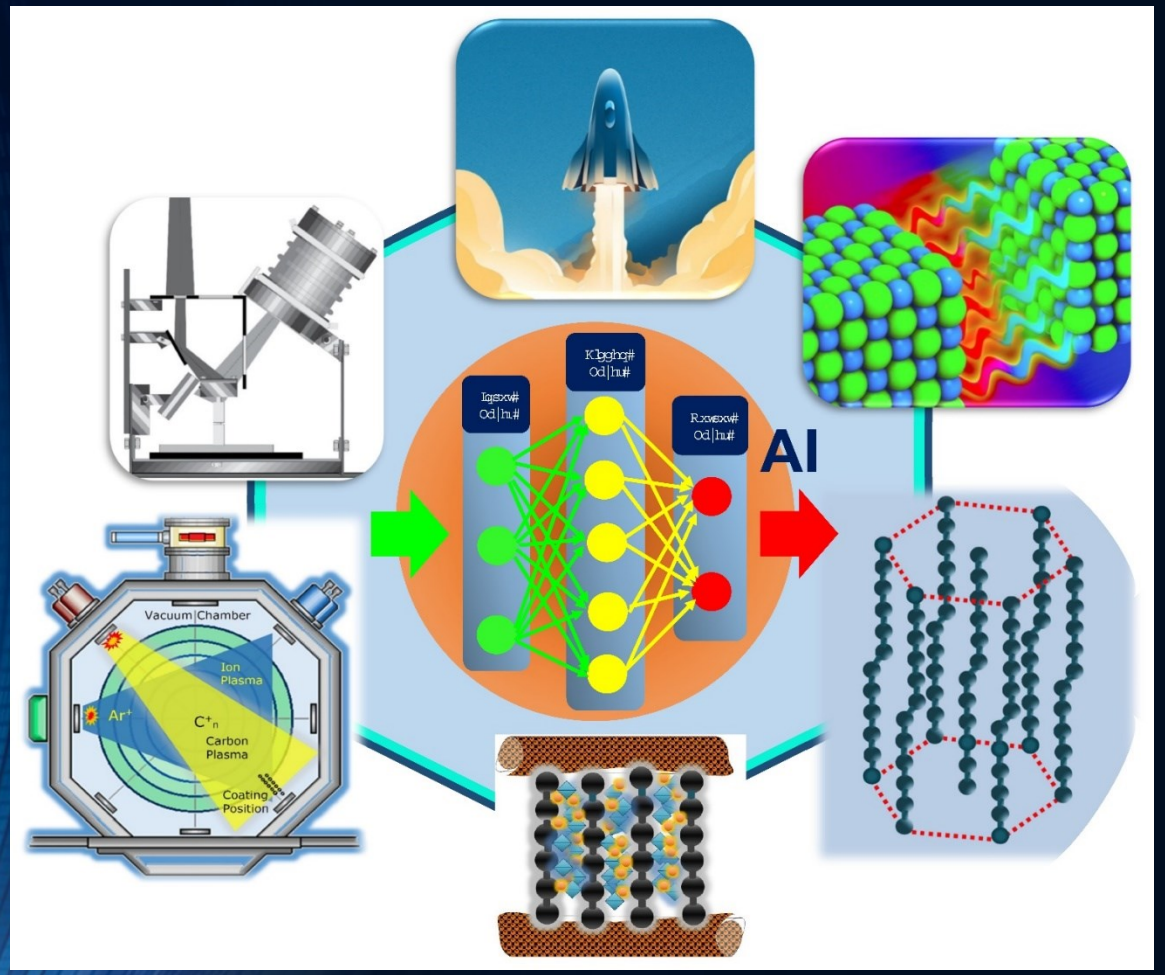
CONCLUSION

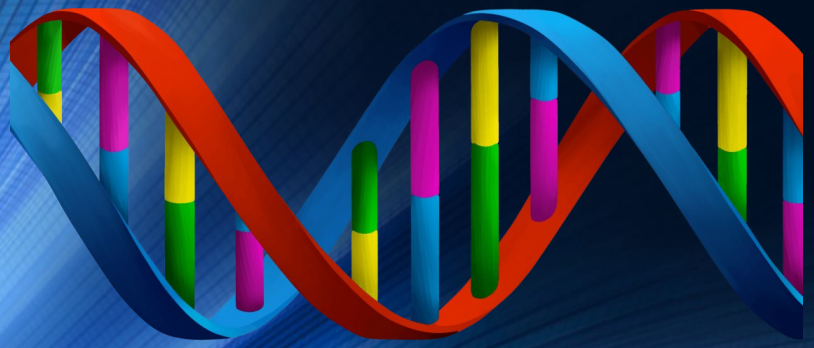
In this presentation, we have demonstrated the significance of a data-driven inverse design strategy for unlocking the latent potential of low-dimensional nanocarbons.
By unraveling hidden growth-properties relationships and identifying universal descriptors, we can precisely tailor the properties and functionalities of nanocarbons.

By analyzing the data-driven nanocarbon genome, researchers can identify previously unknown relationships between the properties of nanocarbon materials. This leads to the creation of new nanomaterials with properties tailored to specific needs, and the potential applications are nearly limitless.

The transformative potential of unlocking the latent capabilities of low-dimensional nanocarbons is substantial. This research breakthrough not only accelerates the development of high-performance materials but also enables advancements in fields like electronics, energy storage, and catalysis.

The data-driven nanocarbon genome is more than just a tool for prediction. It's also a tool for discovery.





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The future is here, and it's data-driven.

Thank you very much for your kind attention!

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Thank you for your kind attention!

Please don't hesitate to contact me if you want to discuss or ask further questions:
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