Technical Note

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

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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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Abstract: Recent advances in the field of nanomaterials have been predominantly influenced by low-dimensional nanocarbon allotropes. Amongst these allotropes, carbyne has garnered significant attention due to its remarkable potential as an authentic one-dimensional carbon chain with sp1 hybridization. In order to maximize the capabilities of this nanomaterial, we utilize a focused data-driven inverse design strategy that relies on the carbon nanomaterial genome approach. This approach acts as a catalyst, allowing us to unlock the untapped potential of nanomaterials. In this approach, a series of multifactorial predictive models based on deep learning neural networks is employed. These models effectively identify universal characteristics that are closely associated with the desired functionalities. As a result, it becomes possible to predict the properties of nanocarbons that are designed in reverse, based on these identified descriptors. The process of utilizing the data-driven carbon nanomaterials genome approach and multifactorial neural network predictive models for the reverse engineering of low-dimensional nanocarbons involves several key steps. These steps include: (i) Gathering a comprehensive dataset that encompasses various growth parameters, modes, and resulting properties of nanostructures; (ii) Conducting thorough data analysis to identify both numerical and categorical descriptors that can serve as informative predictors; (iii) Developing predictive models using deep learning neural networks that effectively capture the connections between these descriptors and the properties of the nanocarbons; (iv) Continuously refining the predictive models based on new insights and information gathered; (v) Employing inverse mapping techniques to determine the required descriptors and growth conditions needed to achieve specific target properties; (vi) Validating the predictive models by synthesizing the nanostructures that were predicted by the models; and (vii) Iteratively enhancing the predictive models by incorporating new validation data and findings. The iterative process of modeling, experimentation, and refinement allows for gradual enhancements in predictive capabilities and precision in inverse design. This data-driven approach, characterized by iterative cycles, helps uncover hidden connections between growth and properties, enabling precise adjustments in low-dimensional nanocarbons to showcase desired structural and functional attributes. The ability to uncover concealed connections between growth mechanisms and resulting properties is crucial for enabling a revolutionary inverse design of low-dimensional nanocarbons. This insight fundamentally transforms our capability to design low-dimensional nanocarbons in reverse, as it provides essential understanding on how to customize synthesis processes to achieve specific desired attributes. In order to expose the vital relationships between growth mechanisms and properties, we introduce a range of innovative technological approaches that serve as catalysts for unlocking the hidden potential of nanomaterials. These methodologies encompass a range of approaches aimed at uncovering the potential of nanomaterials. They involve techniques such as exciting and adjusting synergistic effects, initiating the self-synchronization of collective atomic vibrations within multilayer nano-enhanced interfaces, utilizing the active screen plasma technique, initiating nano-patterns and allotropic phase transformations through energy-driven methods, performing micro/nano-manipulation assisted by surface acoustic waves, introducing heteroatom doping, and achieving directed self-assembly through the application of high-frequency electromagnetic fields. By employing these methodologies, novel neural connections are established within the data-driven carbon nanomaterial genome. The process of observing and modifying significant descriptors and connections is then integrated into our data-driven inverse design approach, as depicted in Figure 1. Innovative technological approaches serve as catalysts, unveiling the latent potential of the data-driven nanocarbon genome. By

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observing and making modifications to descriptors and connections, we can seamlessly integrate them into the inverse design methodology. The knowledge gained from this research holds immense potential to accelerate the discovery of next-generation low-dimensional nanocarbons, characterized by exceptional properties and applications.

Keywords: low-dimensional nanocarbons; machine learning-powered inverse design; data-driven carbon nanomaterials genome approach; deep learning neural networks; multifactorial neural network predictive models; growth-property relationships; universal descriptors; collective atomic vibrations; nano-enhanced interfaces

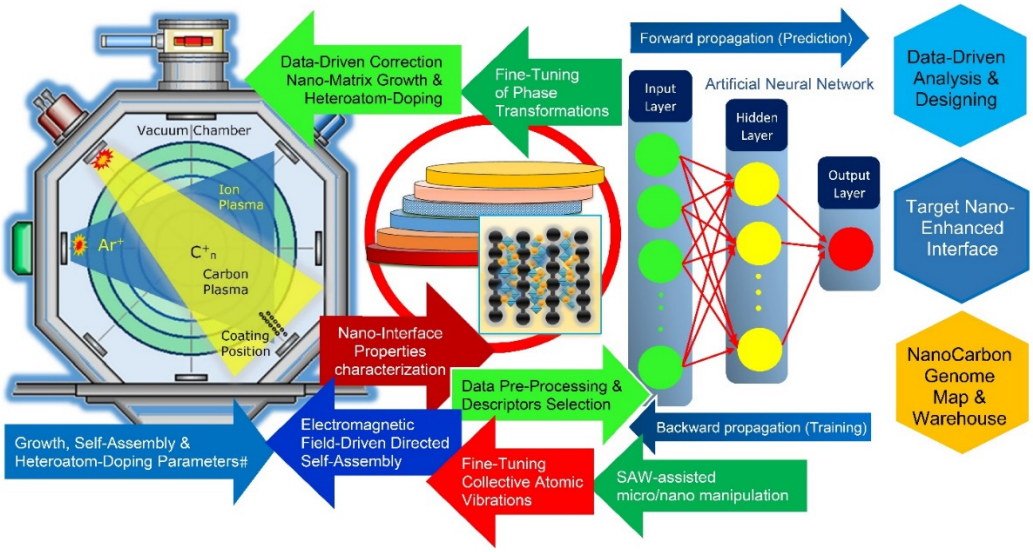

Figure 1. A visual representation showcases the data-based methodology employed to finely adjust and enhance the characteristics of low-dimensional nanocarbons. This systematic approach combines theoretical modeling, precise synthesis, characterization, and machine learning to enable the proactive engineering of low-dimensional nanocarbons through prediction.

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