GrapheNet: A Novel Deep Learning Model for Predicting Physical and Electronic Properties of 2D Materials Using Images

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The quest to represent complex advanced materials and nanostructures has been a persistent challenge in the field of chemistry and materials science. Traditional methods of representing small molecules, such as SMILES, have proven to be insufficient to represent more complex systems. In recent years, the use of 2D images to represent the structure of materials has gained popularity, especially with the development of artificial intelligence (AI) tools and deep learning algorithms [1].

In this study, we present a novel approach to represent the structure of 2D based materials, such as graphene [2] and graphene oxide nanosystems [3], and an advanced predictive AI-based framework. Our proposed deep learning model, GrapheNet, is based on an Inception-ResNet architecture consisting of multiple blocks of convolutional layers with different kernel sizes. The GrapheNet model can be trained to make predictions about the physical and electronic properties of graphene-based systems using PNG images as structural representations. The efficacy of the approach was tested on datasets of graphene oxide and defected graphene systems, built starting from repositories of computed structure/property data. Structural data of the nanosystems in the dataset, encoded in standard structural formats, are transformed into threedimensional (graphene oxide) or two-dimensional (defected graphene) tensors, converted into RGB (graphene oxide) or grayscale (defected graphene) PNG images and pre-processed (cropping, resizing, recentering, padding). Upon training, the GrapheNet framework yielded very accurate results in predicting phyisico-chemical properties of graphene oxide and graphene nanostructures, with low mean prediction errors for all target properties considered, also exhibiting a significant computational efficiency. Being based on highly-efficient frameworks borrowed from state-of-art computer vision technologies, the approach proposed demonstrates the potential of using image-like representations of 2D and low-dimensional nanostructures in connection with deep learning predictive models, predicting the chemico-physical properties of nanographenes with great accuracy and outperforming the computational efficiency of current methods.

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