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Discovery and characterization of advanced materials using Artificial intelligence and precise electronic and chemical imaging techniques

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Advanced materials have contributed significantly and even revolutionized diverse technology and industry fields like information technology, energy, medicine, transportation, environmental science, etc. The significant advances in these areas lead to faster, smaller, more energy-efficient, and more portable systems based on intelligent properties that pave the way for continuously evolving innovative applications. A critical problem in this field is determining the electronic structure of sub-micrometric materials precisely and directly.

Recently, remarkable progress has been achieved in modern microscopies. However, even if they have attained exceptional lateral resolution, the problem of providing a robust spectroscopic and electronic characterization of materials at the nano- and mesoscopic-scale remains. This gap has been recently filled by an innovative and powerful k-space nanoscope or Nano-ARPES (Nano Angle-Resolved Photoelectron Spectroscopy). This cutting-edge nanoimaging technique can determine the momentum and spatial resolved electronic structure, disclosing the implications of heterogeneities and confinement on the valence band electronic states typically present close to the Fermi level. The kspace nanoscope can be effectively combined with chemical imaging based on core levels (and their chemical shifts) scanning photoemission can detect even very tiny different chemical environments. In this presentation, the more relevant Nano-ARPES results will be disclosed [1-7].

In parallel to this powerful experimental approach for materials characterization, recently, there has been an increasing interest in applying Artificial Intelligence (AI) tools [8-9] and their subclasses to better predict novel materials with designed properties. This collection of statistical methods has already obtained considerable success, particularly in the context of the materials genome initiative (MGI) [10]. However, compared to other fields, the materials data are typically much smaller and sometimes more diverse, which undoubtedly affects the construction and effectiveness of AI models. This presentation will describe a deep-learning approach to identify promising candidate energy storage materials. This data-driven method utilizes structural and electronic parameters from the Materials Project, NOMAD, and other available databases. The approach based on a graph neural network (GNN) model trained with a large-prepared dataset will be described, together with the employed

techniques for interpretability and representation analysis. As raw data are vulnerable to noise, corruption, missing, and inconsistent data, pre-processing steps have been carried out using cleaning, integration, transformation, and reduction of the raw data. In some cases, respecting physicochemical criteria, we have also implemented data augmentation approaches to generate data and considerably reduce the error metrics of the used AI techniques.

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