First Principles In Silico Characterisation of Advanced Materials and Bio-Nano Interface

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1. Introduction

Advanced materials (AM) represent a new paradigm in materials science: substances with highly specific features and enhanced target properties derived from precise control over their structure and composition. A particularly relevant set of examples of these materials are nanomaterials, which may exhibit properties that significantly differ from the expected behaviour of the same bulk material due to the high surface-to-volume ratio. The large surface implies high specific reactivity and capacity for steering complex processes at the molecular level. New materials, however, come with new risks: these same desirable properties may also lead to unwanted behaviour when these novel materials come into contact with the environment or living beings. As with the benefits, these risks are high for nanomaterials, since their small size enables rapid uptake by the body through multiple pathways, e.g. inhalation, ingestion, or skin contact. Consequently, it is important to be able to predict whether a given material is toxic or biocompatible early at the stage of the material's development. Given the vast range of materials used in modern technology or considered as candidates for applications, and in light of the general need to reduce the amount of in vivo and in vitro tests performed, this suggests the use of in silico methods to predict complex functionalities of AMs from first principles.

2. Methodology

We present a systematic nanoinformatics approach to generating predictive in silico models of functionalities of AMs. It aims at quantitative description of the materials using a combination of physics-based and data-driven materials modelling methods, focusing on their interfacial properties in complex media. Our multiscale method includes:

- evaluation of detailed properties of the nanomaterial interface with water and parameterization of the atomistic force field for the material using electronic structure methods [1]
- calculation of interactions of the biomolecule building blocks (amino acids, lipid segments, DNA bases) with the surface of the material and interaction between the building blocks at the atomistic level at the specified conditions [2,3]
- parameterization of the coarse-grained (CG) force field for biomaterial building blocks and construction of the sample of arbitrary size and shape [3]
- CG modelling of interaction of entire biomolecules with the nanomaterial surface and calculation of preferred orientation and the mean adsorption energy [1]

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- modelling competitive adsorption of molecules onto NPs and prediction of the biomolecular corona [4]
- generation of NP descriptors covering intrinsic and extrinsic properties [5]
- construction of machine-learning models for the prediction of complex NM functionalities.

In the multiscale scheme, these modelling techniques are coupled to each other thus forming a robust characterization pipeline. The overall concept of the nanoinformatics approach is sketched in Fig. 1.

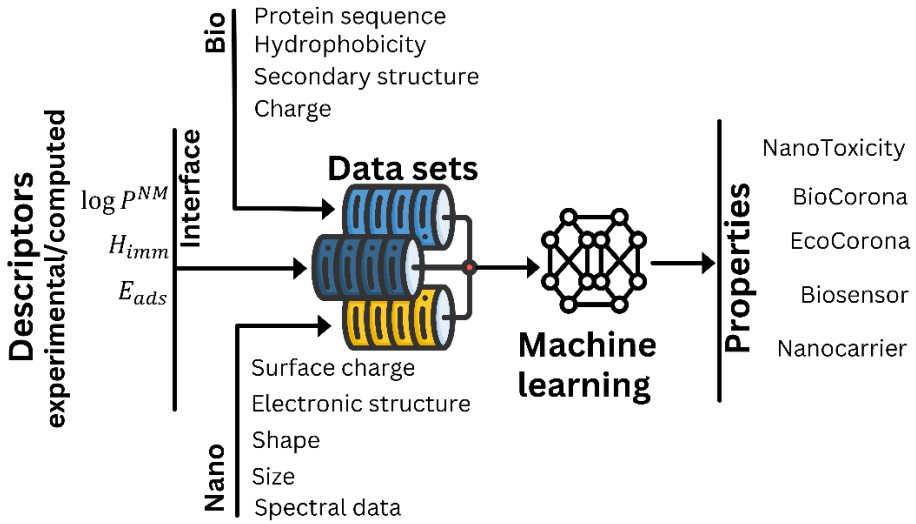

Figure 1: A concept of the nanoinformatics approach combining physics-based and data-driven methods for predicting complex functionalities of AMs [3].

3. Results

We have used the developed theoretical schemes [1-4] to make an open-source software pipeline [6] for in silico AM design and characterisation. In particular, we produced advanced descriptors of multiple common uniform and composite nanomaterials including metals, metal oxides, minerals, carbonaceous materials (carbon nanotubes, graphene, carbon black), polymeric materials and composites. This list features both intrinsic descriptors (ionization potentials, bandgaps, dispersion energy, polarizabilities, dispersion energies) and extrinsic descriptors (immersion enthalpies in water and octanol, adsorption energies for biomolecules, etc.). In this presentation, we demonstrate the outcomes of the advanced in silico characterisation and the predictive power of the nanoinformatics approach using in vitro and in vivo activities of the AMs such as respiratory toxicity or drug delivery.

4. Conclusions

Nanoinformatics approach presents enormous benefits for the modern technology as it allows to screen novel materials for the specific functionality, while saving time and money and avoiding animal experimentation. Although we tested it only in the biomedical field, our methodology is sufficiently flexible to allow for an extension into other applications of AMs and development of safe-and-sustainable-by-design methods

at a fraction of wet-lab costs and brute force materials modelling effort. All the code is available for download from [6] together with a library of required input which covers a wide range of nanomaterials and biomolecules of interest, and further NP materials or adsorbates can be straightforwardly added by the user as required.

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6. References

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