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Editorial

First-Principles Simulation—Nano-Theory

Paolo Restuccia

Department of Chemistry, Imperial College London, 82 Wood Lane, London W12 0BZ, UK; p.restuccia@imperial.ac.uk

First-principles (or ab initio) simulation is one of the most significant theoretical approaches to study and model systems at the atomistic level. Based on solving the fundamental equations of quantum mechanics without any additional assumption or approximation, it has gained relevance in recent decades in many technological fields for materials design and discovery, such as condensed matter physics and nanotechnology, and to unravel macroscopic properties of materials by studying their atomistic and electronic behaviour. The current wide use of first-principles simulations as a predictive and investigative tool is possible due to the higher efficiency of computational resources and the introduction of user-friendly and open-source software packages, which allows performing calculations with hundreds of atoms unfeasible to realise until a few years ago.

This Special Issue on "First-Principles Simulation—Nano-Theory" covers some aspects of the most recent updates about researches involving first-principles simulations. We present eleven original studies investigating phenomena for basic research or technological applications employing state-of-the-art approaches in ab initio calculations.

The first paper by Song et al. [1] focuses on studying structural and photoelectric properties of zincblende InGaN alloys. Through Density Functional Theory (DFT) calculations, the authors discovered that an increased concentration of In atoms leads to a lower bandgap and a redshift in both the imaginary part of the dielectric function and the absorption coefficient, thus enhancing the absorption of visible light and providing theoretical evidence for applying this material in optoelectronic and photovoltaic devices. The study of structural, electronic and optical properties through first-principles simulations is a usual topic also explored by Shafei et al. [2] in their study of kaolinite, muscovite, and montmorillonite crystals, three common clay minerals whose understating of their mechanical properties is essential for their technological applications. Another paper on optoelectronic properties is the one by Liu et al. [3], in which the authors studied through DFT+U simulations how the electronic properties of indium tin oxide films change when the thickness of the film is varied and how this affects the electric resistivity of the material. The study of electronic structure DFT simulations is also performed by Hu et al. [4], where the authors found that the adsorption of 4d transition metal atoms leads to a metallic character in graphene monolayer. Alongside the electronic structure, the analysis of spin states is another widely explored research field in the use of ab initio simulations, as shown by Li et al. [5] in their study of redox magnetism and electrochromism of a cyclometalated triruthenium complex with triarylamine by means of Monte Carlo and DFT calculations, where they found specific spin and adsorption states that suggest the use of this complex as an electrochromic material for electric field detection. First-principles simulations are also used in combination with experiments to unravel the atomistic origin of specific processes, as in the paper by Zhang et al. [6]. The authors performed tribological tests and first-principles calculation of ZrB_2/Mo multilayers to understand the relation between the hardness of this material and its coefficient of friction, finding that the compound stability is the crucial factor to determine its mechanical properties. Sometimes, theoretical calculations provide helpful insights when experimental evidence show conflicting results; this is the case in the paper by Liu et al. [7], where DFT calculations reveal the most favourable adsorption configuration of water molecules on a NaCl(001) surface. It is also possible to calculate reaction and adsorption energies with DFT calculations as in the manuscript by

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Tian et al. [8], where the authors studied the different adsorption behaviour of three pyridine amide additives (Nicotinamide, Pyridine-2-formamide and Pyridine-4-formamide) on Pt(111) surface and found that these molecules react by forming a protective film which avoids the diffusion of atoms to the surface of the growth centre. Cao et al. [9] employed a different approach widely used in the theoretical community: first, they performed classical Molecular Dynamics calculations, which are less computationally expensive, of water impurity in transformer oil; then, they selected specific time frames and local regions to study the electronic properties of the system (such as the density of states and the electron density) and have a clearer picture of the breakdown process of the transformer oil. First-principles simulations allow for performing complex studies involving water/ice systems and their vibrational spectra, as conducted by Yu et al. [10] in their paper where they studied the hydrogen bond vibrations modes of hydrogen-disordered structures of ice, which is a very useful approach for the interpretation of the experimental spectra. Finally, the recent development of high-throughput first-principles techniques widened the possibility of materials design: the paper by Al-Fahdi et al. [11] reports a novel high-throughput framework for creating new carbon allotropes with different mechanical properties and ultrahigh hardness. This approach can be helpful in the future not only for the screening of specific materials properties but also for the discovery of new compounds.

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