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DFT and DFT based Material Databases in the Era of Machine Learning

ABSTRACT

Machine learning has successfully established itself in a variety of industries, ranging from self-driving automobiles to fraud detection. The materials science community has also started to benefit from it. This has been possible because of the available large number of datasets for materials and their properties, created by high-throughput DFT calculations where an automated input can perform thousands of computations in a single shot. Not only DFT has proven to be a very robust tool for understanding the electronic structure but the amount of data it has provided for machine learning based material design is highly valuable.

In the first part of this talk, I will present the use of DFT with an example of e- Fe_2O_3. It is one of the polymorphs of the most abundant material, that is, iron-oxide but least explored due to its metastable state in the bulk form. The magnetic properties such as the spin arrangement, anisotropy as well as the ferroelectric properties like polarization and its switching for the bulk e- Fe_2O_3 will be presented. The stability of thin films and the use of stable thin-film surface for the application of e- Fe_2O_3 in the photoelectrochemical cell will be presented. The stable surface has been hydrolyzed to see the effect of adsorption. The surfaces of the thin-film give rise to the surface states which acts as trapping sites for the electron-hole pairs leading to the loss of charges and a decrease in the efficiency of the devices. To overcome this problem, we have explored the possibility of modelling the heterostructure of two polymorphs, namely α-Fe_2O_3 and e- Fe_2O_3. We find that the alignment of the band edges at the interface of both the materials are such that it gives rise to a rare type- III broken band-gap heterostructure. This heterostructure helps in the charge separation and can result in good PEC device performance.

In the second part of the talk, I will focus on the DFT based databases and their use in predicting material properties using machine learning techniques. Some of the commonly available databases are AFLOWLIB, Materials Project, OQMD, NOMAD, and many more that collect vast quantities of DFT computations in a convenient manner. Use of one such database to understand the magnetic properties of Fe-based compounds will be discussed. The model interpretability and the important role of designing descriptors for better modeling will be presented.

BIO

Dr Arti Kashyap is Associate Professor (Joint Appointment) at IIT Mandi in the School of Physical Sciences and School of Computing. The primary area of her research is to study the magnetic materials using first principles approach and use of big data technologies for various applications including material design. Apart from this, she has a keen interest in socio-technical research areas; specifically in the space where technological intervention can fulfil societal needs.

Dr Arti Kashyap was awarded Simons Associateship from ICTP, Italy in 2015. Very recently she has been selected as one among 75 women in STEAM featured in the book “She Is” by the office of Principal Scientific Adviser, Government of India. Dr Arti Kashyap is Chair of the Women Centre Committee at IIT Mandi and is actively involved in promoting the gender sensitive environment at the institute.

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