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Computational modeling as a complementary and predictive tool in materials science research

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With the recent scenario of affordable computers with large RAM and storage capabilities as well as the availability of high performance computing facilities, research in materials science using ab initio techniques has rapidly grown. The research focus has now gradually shifted from fundamental science investigations to properties of materials that have applications in environmental preservation, search for as well as adoption of alternative fuels and green energy at large, health, among others, which have an expected impact on the quality of life. In the last few years our group has worked on hard materials for cutting and shaping in industry as well as materials for energy conversion and materials for electronic applications. In particular, we have investigated hardness in Transition Metals Carbides and Nitrides (TMCNs) and extended to other indicators such as shear modulus, rigidity and brittleness; metal electrode contacts on diamond surfaces for diamond electronics; metal hydride materials for applications in hydrogen fuel storage and the electronic structure of the interface of dye/TiO2 in dye sensitized solar cells (DSSC), among others. Highlights of the finding of these cases and recent advances are provided. These examples, among others, are provided to show how computational modeling richly supports experimental work and yet can also be used to provide useful information that may not directly be accessible to experiments.

HPC content

Large volumes of data generation for surveys of various combinations of systems to obtain desirable properties

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