Computational Discovery of Sustainable Energy Materials

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Computational Discovery of Sustainable Energy Materials

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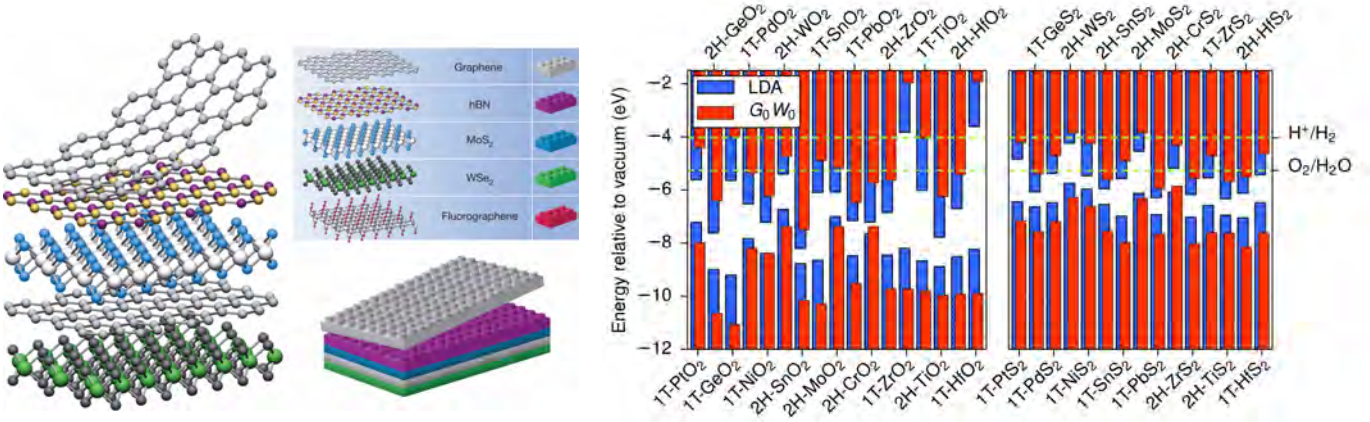
Identifying new high-performance materials is a significant challenge. At present on the order of 200.000 inorganic materials are known. Their chemical composition and crystal structure are stored in crystallographic databases, however, the basic properties (mechanical, electronic, etc.) of these materials remain largely unknown. A systematic, experimental characterization of the properties of this huge set of materials is impossible, but it can be done efficiently and at low cost using modern electronic structure calculations. According to the US Materials Genome Initiative (MGI) and the Materials Science and Engineering Expert Committee, computational materials science will be totally indispensable for materials discovery and design during the next decade. I will review our efforts of employing large-scale quantum mechanical computations to explore and discover new materials for solar energy conversion. Examples will include design of functionalized porphyrins for dye sensitized solar cells(1), novel two-dimensional materials for high performance opto-electronics(2), and perovskites for photo-catalytic water splitting(3). In the spirit of the MGI we contribute to the development of computational property databases that will serve industry and academia in the search for new materials(4).



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