Materials Science

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The main focus in the category "Materials Science" is on families of materials with technological applications or prospects of such in the future. While most may be viewed as a subgroup of "Condensed Matter", it is striking that the overwhelming majority of the projects in "Materials Science" and of those presented in the proceedings of recent NIC-Symposia involve calculations based on the density functional (DF) formalism. This approach allows one to calculate structures and energy differences (including reaction paths) without requiring the input of experimental information. This is a crucial advantage in studies of *families* of related compounds, e.g. what is the effect of exchanging one element with another of the same group? The availability of leadership computers, such as Jugene, has expanded greatly the range of materials *and* the length and time scales accessible to such calculations. Nevertheless, such calculations are still limited to some hundreds of atoms and simulation times of a few hundred picoseconds, and this is a serious restriction for some applications.

The discovery of giant magnetic resonance by Peter Grünberg and Albert Fert led to the award of the 2007 Nobel Prize for Physics and the new field of "spintronics". Here the focus is on changes in magnetic (spin) properties, and it has been a very active area in computational materials science for well over a decade. In the contribution of Atodiresei *et al.* it is coupled with another important development, namely the use of single molecules as "molecular rectifiers", leading to the new field of *molecular electronics*. Calculations have been performed for various organic molecules and graphene on metallic surfaces and provide us with a picture of the the bonding and magnetic properties of these systems. It is interesting that the description of the exchange-correlation energy, an essential ingredient in DF calculations, must be extended to include so-called "van der Waals" attractions between closed shell systems.

Graphene is also an essential part of the contribution by Kiss *et al.* The discovery of single layers of hexagonally bonded carbon atoms led to the award of the 2010 Nobel Prize for Physics to Andre Geim and Konstantin Novoselov and to much excitement among materials scientists. Applications to the real world of electronics still lie in the future, and this paper studies the deposition of graphene-like building blocks in silicon (111) surfaces and predicts that well defined two-dimensional patterns will result.

The ground state magnetic properties of transition metal alloy nanoparticles have been studied using DF calculations, and the results are described in the article by Díaz-Sánchez and Pastor. The size of the clusters (CoRh and CoPt alloys with up to 531 atoms and a diamter of 2 nm) emphasize both the dramatic improvements that have resulted from the

availability of computers such as Jugene *and* the limitations that remain. An application of DF calculations in another context, ion-permeable membranes, is described in the contribution of Lumeij *et al.* We see here how the energy barrier for oxygen hopping in a five-element alloy of Ba, Sr, Co, Fe, and oxygen can be understood, and an additional application is to proton-conducting membranes.

Phase change materials form the basis of many familiar rewriteable storage devices, including DVD-RW, DVD-RAM, and the Blu-ray Disc. The information is stored in very thin layers of an alloy in microscopic "bits" that can switch rapidly and reversibly between the amorphous and crystalline states. The article by Akola and Jones describes a detailed DF study of the amorphous structure of an alloy of Ag/In/Sb/Te that has found widespread use in the DVD-RW world. It is still not possible to simulate the crystallization for such an alloy for samples with hundreds of atoms, but the work has led to a plausible picture of the process that can be studied further.

The remaining application described here requires far larger samples and longer time scales than are currently accessible to DF calculations. Pastewka and Moseler describe molecular dynamics simulations of friction properties of hydrogenated diamond-like carbon films under high pressure. The hydrogen concentration of such films plays a crucial role in determining these properties.

These short articles provide just a sample of the wide range of materials properties being studied using the facilities of NIC. Much of this work seeks answers to problems originating in technological applications, and there will be many challenging problems in this field for years to come. There is no doubt that the coming generations of supercomputers, as well as the development of new algorithms and programming techniques, will play crucial roles in finding the solutions.