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Materials Science

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The science of materials has benefited immensely from the rapid improvement of computer hardware and numerical algorithms. Today it is possible to calculate structural, cohesive, and magnetic properties for complex systems with many atoms without using any information from experiment. It is also possible to perform calculations simultaneously on many smaller, but important systems in the time taken by one such calculation only a few years ago. Such calculations can provide information about the properties of materials, such as the motion of individual atoms, that is often unattainable by any other means. Radioactive, poisonous, and short-lived atoms and molecular complexes present no special problems. All this is true, in particular, for calculations using the density functional (DF) formalism, which is the basis of most calculations in condensed matter physics that have no adjustable parameters, and it has become an indispensable tool in theoretical chemistry. The following contributions provide examples of how density functional and other calculations can provide insight into important materials.

The electronic properties of interfaces present particular challenges, and three of the case studies are from this area. Silicon carbide (SiC) is a wide-bandgap semiconductor with remarkable structural and electronic properties in the bulk and at interfaces. The work by Peng et al. focuses on the structure of (001) surfaces of SiC and the nature of its reconstruction. The extension to the adsorption of acetylene (C_2H_2) on the SiC(001)-(2×1) surface has also been carried out. The hydrogen induced metallization of SiC surfaces has been studied in the case of the (001)-(3×2) surface. Surface and adsorbate structures are also the focus of Stekolnikov et al., who investigate the Si(111) surface, one of the best studied of all. This surface shows some remarkable quasi-1D structures when indium is adsorbed on it, and different structures lead to band structures that have gaps or can show metallic behaviour. Spin-polarized density functional calculations indicate that there is only a weak tendency for spin ordering on reconstruction. Spin-polarized DF calculations are, of course, essential in calculations involving magnetic properties, and these have been performed by Bihlmayer et al. for several systems with complex magnetic ground states. The systems studied include ultra-thin magnetic films and nanowires on stepped surfaces. In collaboration with experimental groups, such calculations will be invaluable in aiding the development of new devices.

The work of Entel et al. also uses spin-polarized DF calculations and focuses on other materials of technological importance, namely alloys that exhibit magnetic shape memory. These calculations provide insight into the reasons for stability (and instability) in Heusler alloys. Semiconductor quantum dots (QD) are the subject of the remaining contribution (Lorke et al.). The strong interaction between carriers and phonons in these systems requires a description in terms of polarons, and these authors have performed a quantum-kinetic calculation to study the efficiency of different scattering processes and the way they affect the optical spectra.

These contributions give but a sample of the rich variety of materials problems that are carried out on the supercomputers of the John von Neumann Institute for Computing. In spite of the range and complexity of these applications and the insight obtained from them, it should be noted that they are very demanding of computer resources. There are many phenomena that involve even larger length and time scales than are currently accessible using present computers, and much development in hardware and numerical algorithms will be needed before we can describe the details of such extended systems.