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Computer simulations provide information about the properties of materials that is often unattainable by any other means. It is not only possible to obtain information about the coordinates and motion of individual atoms, but there is no difficulty in dealing with radioactive, poisonous, or short-lived species. The availability of high-performance supercomputers in recent years has expanded the scope of such simulations greatly. This is particularly true for so-called "first principles" methods, which seek to determine structural, cohesive, and magnetic properties of materials without recourse to data obtained from experiment. Density functional calculations provide an example of such methods.

The density functional formalism is the basis of all almost calculations without adjustable parameters in condensed matter physics, and the last decade has also seen its establishment as an indispensable tool in theoretical chemistry. Materials scientists are usually interested in obtaining detailed information about complicated systems, and they have benefited greatly from recent developments in hardware and in numerical algorithms. In the following three contributions we see examples of how density functional calculations can provide insight into important materials.

Clusters[a] of atoms have properties that are quite distinct from bulk systems, and the development of experimental techniques in the past 20 years has provided many challenges to theorists. The contribution by Moseler shows how a combination of density functional methods with molecular dynamics - in particular, using a time-dependent formulation - can provide us with optical and photoelectron spectra of Na clusters. Results are also provided for the structures of anions of clusters of Cu, Ag, and Au, as well as the interaction between Pd clusters and an MgO surface. Supercell calculations of alkali atoms intercalated in transition metal chalcogenides, such as $TiTe_2$, are described by Schattke and Ramírez. Finally, Dąbrowski and Zavodinsky discuss the effects of point defects in Pr oxides, and on the structure and formation of the interface between these oxides and SiO_2.

In spite of the range and complexity of these applications and the insight obtained from them, we must note that they are very demanding of computer resources. Much development in both hardware and software will be necessary before we can describe extended systems over the long time scales necessary to describe some phenomena.

[a] Cluster: "a compact group of other similar things", The New Shorter Oxford English Dictionary, Clarendon Press, Oxford (1993).