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It has almost become a cliché to observe that materials science is one of the great beneficiaries of changes in the landscape of scientific computing. The increase of computing power of several orders of magnitude over the past 20 years has been accompanied by improved methods and algorithms that allow us to calculate structural, cohesive, and magnetic properties of systems of many atoms and several elements without using any input from experiment. Furthermore, it is possible to perform calculations simultaneously on families of materials in the time required for a single system only a decade ago. In amorphous and other disordered systems, to mention just one example, the motion of individual atoms can be calculated in a detail that is often unattainable by experimental means. Of course, radioactivity and poisonous materials present no special problems for computer simulations. The density functional (DF) formalism is the basis of most calculations in condensed matter physics that have no adjustable parameters, and its early development led to the award of the Nobel Prize in Chemistry in 1998. The DF theory is the basis of the five materials science contributions in this volume.

I am writing these lines on the day that Albert Fert and Peter Grünberg were awarded the 2007 Nobel Prize for Physics for their discovery of giant magnetic resonance (GMR). The change in resistivity of multilayer structures caused by an external magnetic field is the most spectacular (and technologically the most successful) example of *spintronics*. In their contribution, Bergqvist and Dederichs discuss possible future applications in this area based on dilute magnetic semiconductors, such as $Ga_{1-x}Mn_xAs$. Their focus is on the critical behaviour, and they combine the DF method to determine the exchange interactions in a model system that is then studied with Monte Carlo statistical methods. Magnetic properties are also discussed in the paper of Gruner, Rollmann, and Entel, who studied clusters of hundreds of transition element atoms. Their results for Fe_{561} and for Fe-Pt and Co-Pt alloys indicate that calculations for 1000-2000 atom systems are certainly feasible in the near future.

Magnetic storage in computers is so familiar that we may think that there are no alternatives. This is not the case. All users of personal computers must have wondered about (and annoyed by) the delay between switching on a PC and it becoming operational. The reason is that normal random access memory (RAM) is "volatile", i.e. the content vanishes when power is switched off, and the operating system must be "booted" from the hard disk. Non-volatile memory is familiar to us in the form of USB sticks and memories used in digital cameras, but the limitations of such "flash memory" in scaling to smaller dimensions have stimulated the search for highly stable, high density alternatives. The materials of choice at the moment are tellurium-based alloys, and some of the most interesting are discussed in the article by Jaakko Akola and me.

For as long as I can remember, electronic structure calculations have promised to deliver detailed understanding of heterogeneous catalysis, without doubt an area of huge technological importance. The contribution of Huber *et al.* shows that we have made much progress along this path. Their focus is on the structure of palladium clusters (and their oxides) located on magnesium oxide surfaces. This work provides a further example of the ways in which detailed calculations aid the interpretation of experimental data. The final contribution to this section (by Ramos and Bechstedt) provides an example of how "standard" density functional calculations, which provide us with geometrical structures and cohesive properties, can be extended to properties of excited states, such as optical properties. This can be done by the *GW approximation* to the self-energy of the systems, which in this case are nanocrystallites of germanium and silicon with several hundred atoms and an array of defects.

The applications described in this section are just examples of materials science projects that are carried out on the supercomputers of NIC (JUMP and JUBL). Calculations on large clusters for simulation times that were unthinkable a few years ago are becoming almost routine, and the coming generations of computers conjure up prospects that are even more exciting. The techniques developed by scientists to study properties of the "materials" world have reached, for example, systems whose sizes are relevant for reactions involving biological molecules. Perhaps the biologists should watch out for us!