Psi-k 2005: Some Remarks by the Conference Chairman

In the two months after the Psi-k 2005 Conference in Schwäbisch Gmund there has been some time to reflect more on scientific contents of the meeting and the message it delivered about the state of our field.

The first observation concerns the *diversity* of scientific questions now addressed by electronic-structure calculations. Heterogeneous catalysis and other surface reactions have long been in the repertoire of our community and continue to flourish. The same is true for metallic alloys and other structural materials, but we now see major efforts also in first-principles calculations for interface structures, for biological matter and biological processes, and for geophysics and earth sciences.

Quantum transport is another area where there has been major growth in the exploitation of electronic-structure methods. Density-functional theory can provide a realistic Hamiltonian to be plugged into the powerful methods developed in the mesoscopic-transport community. Devices based on nanoscale structures, ranging from single molecules attached to external leads to nanowires and ultrathin insulator layers, are now subject to quantitative modelling. Quantum transport in atomic-scale structures opens up also theoretical challenges, as it is not exactly clear what is the range of validity for the Landauer-type methods. Many-electron correlations, inelastic effects, and explicit time dependence are interesting topics now under intensive study.
The diversity also includes extensive work on quantum dots, rings and other nanostructures, where quantum confinement effects influence the physical properties, such as optical and other excitation spectra. Again, DFT methods can provide the benchmarks for small systems, which can be scaled up for investigations of the structural and electronic properties of large (million-atom) assemblies using simplified model Hamiltonians. There are also many other areas of nanoscience, where computational methods provide decisive input and insight, including nanomechanical phenomena and growth by self-assembly.

Nanoscale and complex magnetism is an exciting area where computational methods have shown their power. Magnetic ordering in thin films and superlattices has enormous technological potential, and new magnetic materials (such as multiferroics) are intensively explored. Spin switching, spin-transfer torque and the Rashba effect are examples of current topics in magnetoelectronics, another technologically interesting and rapidly expanding area. Intensive work continues in the search for useful materials for spintronics, such as dilute magnetic semiconductors. Their properties are sensitive to the presence of defects and impurities, which need to be understood in great detail.

Let me round up the diversity argument by noting the progress made in first-principles approaches to superconducting materials. For many superconducting materials, the devil is in the details of the complex system, as both electronic properties and electron-phonon interactions depend critically on the atomic-scale composition and structure.

The second observation are the strong advances made in quantitative understanding of many-electron effects. It has long been known that these are important for strongly correlated materials, and that the mean-field description of standard DFT cannot treat them properly. On the other hand, the model Hamiltonians popular in many-body theories often fail to

describe the real physical system of interest, or contain parameters that need to be adjusted. It has now become possible to intertwine many-electron theories and faithful atomic-scale description into a first-principles approach. A remarkable symposium on ab initio quantum many-body calculations ran through the whole Psi-k 2005 Conference. It brought together the practitioners of several approaches to the problems, such as dynamical mean-field theory, many-body perturbation theory, quantum Monte Carlo methods, and time-dependent current-density functional theory. For those who had the chance to follow these sessions during the conference, this provided a unique overview of the impressive development in both fundamental theories and applications to specific systems. The incorporation of these methods into everyday electronic-structure codes is now happening fast. It seems that in near future "beyond-LDA" or "beyond-GGA" methods will be almost routine, as it is becoming possible to overcome the technical and computational limitations. This is a truly remarkable development and opens many new possibilities for predictive work. The computational demands are strong, however, and for accurate descriptions of, say, van der Waals interactions in extensive systems, additional shortcuts should be explored.

This leads me to my third observation, concerning the vigorous development of new computationally efficient methods. Linear-scaling DFT codes have made impressive progress, which is also evident in quantum Monte Carlo methods. Molecular-dynamics and hybrid methods combining quantum mechanics with classical force fields are applied to demanding problems, for example in soft-matter and solvent systems. Time-dependent DFT methods and transport codes profilerate and are being commercialized. The workhorse DFT codes keep on adding features and functionalities and are also coupled to databases with structural and physicochemical information.

The much improved availability and documentation of electronic-structure and related computer codes have facilitated there widespread use also beyond academia. This is reflected in my final observation: the large number of industrially relevant, "dirty" real-world problems now being at least in part solved by the methods developed in and known to the Psi-k community. There is little doubt that "our" methods are now making a strong impact in applied research and technical development and have become an important tool for industrial research. We should all feel proud and encouraged by this.

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Psi-k 2005 Chairman