

# Toward Computational Materials Design: The Impact of Density Functional Theory on Materials Research

Jürgen Hafner, Christopher Wolverton, and Gerbrand Ceder, Guest Editors

## Abstract

The development of modern materials science has led to a growing need to understand the phenomena determining the properties of materials and processes on an atomistic level. The interactions between atoms and electrons are governed by the laws of quantum mechanics; hence, accurate and efficient techniques for solving the basic quantum-mechanical equations for complex many-atom, many-electron systems must be developed. Density functional theory (DFT) marks a decisive breakthrough in these efforts, and in the past decade DFT has had a rapidly growing impact not only on fundamental but also industrial research. This article discusses the fundamental principles of DFT and the highly efficient computational tools that have been developed for its application to complex problems in materials science. Also highlighted are state-of-the-art applications in many areas of materials research, such as structural materials, catalysis and surface science, nanomaterials, and biomaterials and geophysics.

**Keywords:** computation, density functional theory, modeling, nanoscale, simulation.

## Introduction

During the past decade, computer simulations based on a quantum-mechanical description of the interactions between electrons and atomic nuclei have had an increasingly important impact on materials science, not only in fundamental understanding but also with a strong emphasis toward materials design for future technologies. The simulations are performed with atomistic detail by solving the Schrödinger equation to obtain energies and forces, require only the atomic numbers of the constituents as input, and should describe the bonding between the atoms with high accuracy. The Schrödinger

equation for the complex many-atom, many-electron system is not analytically solvable, and numerical approaches have become invaluable for physics, chemistry, and materials science. A breakthrough in these computational efforts was realized in 1964 when Walter Kohn and co-workers developed the density functional theory (DFT), a theory based on electron density, which is a function of only three spatial coordinates.<sup>1</sup> The Kohn–Sham equations of DFT cast the intractable complexity of the electron–electron interactions into an effective single-particle potential determined by the exchange–correlation

functional. This functional (i.e., a function whose argument is another function) describes the complex kinetic and energetic interactions of an electron with other electrons. Although the form of this functional that would make the reformulation of the many-body Schrödinger equation exact is unknown, approximate functionals have proven highly successful in describing many material properties.

Efficient algorithms devised for solving the Kohn–Sham equations have been implemented in increasingly sophisticated codes, tremendously boosting the application of DFT methods. New doors are opening to innovative research on materials across physics, chemistry, materials science, surface science, and nanotechnology, and extending even to earth sciences and molecular biology. The impact of this fascinating development has not been restricted to academia, as DFT techniques also find application in many different areas of industrial research. The development is so fast that many current applications could not have been realized three years ago and were hardly dreamed of five years ago.

The articles collected in this issue of *MRS Bulletin* present a few of these success stories. However, even if the computational tools necessary for performing complex quantum-mechanical calculations relevant to real materials problems are now readily available, designing a series of simulations that meaningfully represent a physical or chemical property or model a process (e.g., a chemical reaction or phase transformation in a material), remains a challenging task, requiring a judicious choice of approximations and an expert handling of these tools.

## Designing DFT Calculations for Materials Science

The successful application of DFT to a materials problem involves three distinct steps: (1) translation of the engineering problem to a computable atomistic model, (2) computation of the required physico-chemical properties, and (3) validation of the simulation results by confrontation with laboratory experiments.

## Translation

A theory that relates computable quantities to macroscopic engineering behavior is a prerequisite in order for DFT calculations to be relevant. Before any computation can be started, significant effort often must be expended to translate an engineering problem into questions and challenges that can be addressed with DFT. This initial step requires considerable insight into the materials science and engineering aspects of the problem.

The translation step may be illustrated by the application of DFT to the design of better materials for rechargeable lithium batteries. Some properties, such as the electrode potential for a new material, can be directly related to total energy differences<sup>2</sup> and are therefore easy to compute. But another critical property, such as cycle life (the loss of capacity after repeated charge and discharge), is more difficult to predict with DFT, because it can be caused by a variety of poorly identified phenomena, such as reaction of the material with the electrolyte to form an insulating layer, mechanical degradation with resulting loss of electrical contact, and phase transformations in the material. Each of these factors requires a different computation.

## Computation

In many cases, solving the Schrödinger equation is not enough. The length and time scales accessible by DFT calculations are defined by the maximal system size (typically a few hundred atoms; up to a few thousand in special cases) and by the maximum time span that can be covered by *ab initio* molecular dynamics (MD) simulations (several tens of picoseconds). A strategy of multiscale simulations must be used to translate the results of atomistic DFT simulations to real-world scales. As an example, the elementary steps in the catalytic oxidation of CO on a metallic surface (adsorption/desorption/diffusion of CO and O<sub>2</sub>, surface oxidation, dissociation of oxygen, reaction CO + O → CO<sub>2</sub>, desorption of CO<sub>2</sub>, etc.) at fixed chemical potentials of the reactants may be treated by DFT calculations, and the results must be fed into kinetic Monte Carlo simulations to develop a comprehensive picture of the reaction under realistic pressure conditions and at real time scales (see also the article by Nørskov et al. on catalysis in this issue).

## Validation

After DFT computations are performed, validation is an important step. This requires going beyond the computation of energies, band structures, and atomic configurations to the calculation of experimentally accessible properties such as mechanical or thermodynamic properties and electronic or vibrational spectra.

Discrepancies between computation and experimental observation can be attributable to inaccuracies in the DFT approach, but more often point to discrepancies between the experimental and computational situations. An experimental result may be influenced by impurities not accounted for in the computation, it may be kinetically constrained, or it may

differ from the computed result because of other factors that are not characterized well in the problem translation. However, it should be emphasized that one of the most important roles of computational modeling is to provide information that is not accessible (or accessible only with great difficulty) by laboratory experiments.

## Hierarchy of Exchange-Correlation Functionals for DFT

DFT reformulates the many-body Schrödinger equation in the form of a set of coupled one-electron equations (the Kohn–Sham equations), where all of the many-body interactions are contained in the exchange-correlation functional

$$E_{xc}[n(\vec{r})], \quad (1)$$

where  $n(\vec{r})$  is the electron density distribution in the crystal. (For a modern introduction into DFT, see, for example, Dreizler and Gross<sup>3</sup> or the recent book by Martin,<sup>4</sup> which also provides a thorough introduction to the theory and practice of electronic structure calculations.) However, the exact form of this functional for which the Kohn–Sham equations would give exactly the same ground-state answer as the many-body Schrödinger equation is not known, and approximations must be used. Perdew<sup>5</sup> has referred to the hierarchy of approximations developed during the last two decades as the “Jacob’s ladder of DFT.”

■ In the local density approximation (LDA), the local exchange-correlation energy density is taken to be the same as in a uniform electron gas of the same density. Modern forms of the LDA are based on the total energy of the homogeneous electron gas derived from quantum Monte Carlo calculations.

■ The generalized gradient approximation (GGA) introduces a dependence of  $E_{xc}$  on the local gradient of the electron density,  $|\nabla n(\vec{r})|$ . Many different forms of GGA functionals are available in the literature, but for materials simulations, it is good practice to use parameter-free functionals derived from known expansion coefficients and sum rules of many-body theory<sup>6,7</sup> and to avoid empirical parameterizations popular in molecular quantum chemistry.

■ Meta-GGA functionals use the kinetic energy density (or the Laplacian of the electron density) as an additional variable.<sup>8</sup>

■ Hyper-GGA uses Kohn–Sham one-electron wavefunctions (instead of the many-body wavefunctions) to evaluate the Hartree–Fock exchange formula; this is commonly called “exact” exchange.

■ Hybrid functionals<sup>9,10</sup> mix exact (i.e., Hartree–Fock) and DFT exchange.

LDA and GGA are by far the most commonly used functionals today. All functionals exist in spin-degenerate and spin-polarized versions. Quite generally, GGA calculations represent a systematic improvement, compared with the LDA, although for heavy elements, a certain tendency of the GGA to overcorrect the LDA error is observed. In certain cases (prominent examples are the structural and magnetic ground state of iron and the potential-energy landscape for molecular dissociation on a metal surface) the difference is not merely a quantitative one: only GGA calculations<sup>11</sup> predict iron to be bcc and magnetic, whereas the LDA predicts the ground state to be hexagonal and non-magnetic. Only GGA calculations lead to the correct height and location of the dissociation barrier for a diatomic molecule in contact with the surface of a metal.<sup>12</sup> Climbing the density functional ladder further to the meta-GGA or hyper-GGA leads to only moderate progress, compared with the GGA.<sup>13</sup> Hybrid functionals enjoy enormous popularity in molecular chemistry, but in materials science they are merely at the test stage. Preliminary results show great promise for insulating and semiconducting systems, but also show a need to develop new hybrid functionals better suited to describing metals.<sup>14</sup>

## Basis Sets

Practically, the effective one-electron Kohn–Sham equations are nonlinear partial differential equations that are iteratively solved by representing the electronic wave functions by a linear combination of a set of basis functions. Basis sets fall into two classes: plane-wave basis sets and local basis sets. Basis-set convergence is crucial for the accuracy of the calculations—in particular, for the prediction of pressure, stresses, and forces.

## Plane-Wave Basis Sets: Calculating Accurate Forces and Stresses

Basis-set convergence is easily controlled in calculations using plane-wave basis sets; it is sufficient to monitor the evolution of the results with the cut-off energy, the highest kinetic energy associated with a plane wave. However, to achieve convergence at a tractable computational effort, the plane-wave basis set must be either augmented by solutions of the radial Schrödinger equation in a region surrounding the nucleus (a modern approach following this line is the full-potential linearized augmented plane-wave method, LAPW) or by using pseudopotentials to describe the electron–ion interaction. A particular advantage of plane-wave calculations is that the calculation of forces acting

on the atoms and stresses on the unit cell is straightforward with the Hellmann–Feynman theorem. This opens the route to quantum *ab initio* MD simulations studying the time development of a system.

## Local Basis Sets: Toward Linear Scaling

Basis-set convergence is much more difficult to control if local basis functions (for example, atom-centered orbitals in a linear combination of atomic orbitals, or LCAO) are used. These approaches have been actively pursued as, in principle, a much smaller basis set; typically 10 to 20 basis functions per atom should be sufficient to achieve the same accuracy as plane-wave calculations using hundreds of plane waves per atom. However, very recent extended tests have questioned that advantage, indicating that to match the accuracy of fully converged plane-wave calculations, very large local basis sets are required.<sup>14</sup> A specific advantage of local basis sets is that they enable the implementation of linear-scaling DFT methods (i.e., algorithms for which the computational effort increases linearly with the number of atoms).<sup>15–17</sup> These techniques rely on the fact that the wave function may be localized and have an exponential decay leading to a sparse Hamiltonian.

For molecular, insulating, and semiconducting systems, linear-scaling, or  $O(N)$ , techniques enable the performance of atomistic studies for systems containing thousands of atoms. However, this does not hold if the gap between occupied and empty states vanishes, as in metals, for which it has turned out to be difficult to reconcile linear scaling and high accuracy.

## Potentials and Pseudopotentials

Methods using local basis sets or augmented plane waves may be constructed as all-electron methods in the sense that the effective one-electron potential is calculated using the full set of relaxed core and valence orbitals. In plane-wave calculations, the electron–ion interactions must be described by a pseudopotential, eliminating the need for an explicit treatment of the strongly bound and chemically inert core electrons. Pseudopotentials may also be used in local orbital methods to reduce the computational effort. The theory of pseudopotentials is mature, but the practice of constructing transferable and efficient pseudopotentials is far from straightforward. Methods for generating pseudopotentials include the pseudopotentials by Troullier and Martins<sup>18</sup> (conserving the norm of the wave function) and the ultrasoft pseudopotentials introduced

by Vanderbilt<sup>19</sup> (which have the merit of making calculations for *d*- and *f*-electron metals feasible at an acceptable computation cost). The criterion for the quality of a pseudopotential is not how well the calculation matches experiment, but how well it reproduces the result of accurate all-electron calculations. Mature codes (see Table I) provide extensive databases of well-tested pseudopotentials. A certain drawback of pseudopotential calculations is that because of the nonlinearity of the exchange interaction between valence and core electrons, elaborate nonlinear core corrections are required in all systems where the overlap between the valence- and core-electron densities is not completely negligible. The projector-augmented wave (PAW) method proposed by Blöchl<sup>20</sup> and adapted by Kresse and Joubert<sup>21</sup> avoids the necessity of core corrections and combines the efficiency of pseudopotentials with the accuracy of full-potential, all-electron calculations.

## Codes

A variety of mature DFT codes are nowadays available to the materials science community. Some of them are accessible through general public licenses, whereas others are proprietary. The codes are based on different choices of

**Table I: Commercially or Freely Available Density Functional Theory Codes.**

Code Name	Basis Set	Potentials	Web Site
<b>Plane Wave Pseudopotential Codes</b>			
ABINIT	Plane wave	Pseudo, PAW <sup>a</sup>	<a href="http://www.abinit.org">www.abinit.org</a>
CASTEP	Plane wave	Pseudo	<a href="http://www.tcm.phy.cam.ac.uk/castep/">www.tcm.phy.cam.ac.uk/castep/</a>
CPMD	Plane wave	Pseudo	<a href="http://www.cpmid.org/">www.cpmid.org/</a>
Dacapo	Plane wave	Pseudo	<a href="http://dcwww.camp.dtu.dk/campos/Dacapo/">dcwww.camp.dtu.dk/campos/Dacapo/</a>
FHlmd	Plane wave	Pseudo	<a href="http://www.fhi-berlin.mpg.de/th/fhimd/">www.fhi-berlin.mpg.de/th/fhimd/</a>
PWscf	Plane wave	Pseudo	<a href="http://www.pwscf.org/">www.pwscf.org/</a>
VASP	Plane wave	Pseudo, PAW	<a href="http://cms.mpi.univie.ac.at/vasp">cms.mpi.univie.ac.at/vasp</a>
<b>Pseudopotential Codes with Other Basis Sets</b>			
Quickstep	Gaussian + plane wave	Pseudo	<a href="http://cp2k.berlios.de/quickstep.html">cp2k.berlios.de/quickstep.html</a>
SIESTA	Local/numerical	Pseudo	<a href="http://www.uam.es/departamentos/ciencias/fismateriac/siesta/">www.uam.es/departamentos/ciencias/fismateriac/siesta/</a>
<b>All-Electron Codes</b>			
CRYSTAL	Local	all-electron	<a href="http://www.crystal.unit.it">www.crystal.unit.it</a>
FPLO	Local	all-electron	<a href="http://www.ifw-dresden.de/agtheo/FPLO/">www.ifw-dresden.de/agtheo/FPLO/</a>
Gaussian 03	Local	all-electron	<a href="http://www.gaussian.com">www.gaussian.com</a>
ADF	Local	all-electron	<a href="http://www.scm.com">www.scm.com</a>
DMol <sup>3</sup>	Local/numerical	all-electron	<a href="http://people.web.psi.ch/delley/dmol3.html">people.web.psi.ch/delley/dmol3.html</a>
FLAIR	LAPW <sup>b</sup>	all-electron	<a href="http://www.uwm.edu/~weinert/flair.html">www.uwm.edu/~weinert/flair.html</a>
QMD-FLAPW	LAPW	all-electron	<a href="http://flapw.com">flapw.com</a>
WIEN2K	LAPW	all-electron	<a href="http://www.wien2k.at">www.wien2k.at</a>

<sup>a</sup>PAW = projector-augmented wave method.

<sup>b</sup>LAPW = linearized augmented plane-wave method.

basis sets, potentials, exchange-correlation functionals, and algorithms for solving the Schrödinger equation. A summary of many existing codes is given in Table I. There are currently a large number of pseudopotential codes, all of which have LDA and GGA functionals and enable the performance of static electronic structure and total energy calculations as well as *ab initio* MD simulations, using either Born–Oppenheimer or Car–Parrinello dynamics. The all-electron PAW method is implemented in VASP and ABINIT codes. Exact exchange and hybrid functionals are implemented in the newest releases of CPMD and VASP. For the pseudopotential codes, an important point is the availability of thoroughly tested, accurate, and efficient pseudopotentials for all elements. Many of these codes come with suites of pseudopotentials developed and recommended by the code developer.

All-electron codes exist using local or augmented plane-wave basis sets. Both Gaussian 03 and CRYSTAL can perform DFT, exact exchange, and hybrid calculations, and FPLO is a fully relativistic code for solving the Dirac equation. DMol<sup>3</sup> uses a numerical basis set working either in an all-electron mode or using semilocal pseudopotentials. WIEN2K, FLAIR, and QMD-FLAPW are all-electron codes using the full-potential LAPW method. WIEN2K offers the ability to add local orbitals to the basis set to speed up convergence. All-electron codes are important for providing benchmarks for pseudopotential codes; this applies in particular to the full-potential LAPW method in which the augmented plane-wave basis provides an efficient control of basis-set convergence.

Today, calculations with tens of atoms are extremely fast, with pseudopotential as well as all-electron codes. Calculations for unit cells containing a few hundred atoms are routine with pseudopotential and PAW codes, but are very demanding or even out of reach for most all-electron codes. Using the most efficient codes, very accurate calculations involving a thousand or more atoms are possible (it should be pointed out that the real figure of merit is the number of valence electrons—the current limit is somewhere close to 10<sup>4</sup> electrons). Linear-scaling calculations may be extended to several thousands of atoms.

## Tools and Capabilities

For many applications in materials science, the availability of a basic code for solving the Schrödinger equation is not sufficient; the resulting energies, wave functions, and electron and spin densities are merely the starting point for the calculations of many different materials

properties. Much current code development is focused on the development of routines for the post-processing of DFT results (“tools”) to yield a comprehensive description of materials and dynamic modeling of time-dependent processes in materials. Examples of such capabilities include

1. Crystal structure, phase stability, and phase diagrams. Whereas the calculation of structural free-energy differences for polytypes of ordered crystalline materials is a standard task within DFT, the combination of *ab initio* total energy calculations with genetic algorithms<sup>22,23</sup> is leading to the development of a truly predictive computational crystallography.

2. Mechanical properties. Symmetry-general techniques have been developed for the calculation of elastic constants.<sup>24</sup> Intense efforts are being made to calculate tensile and shear strength and to simulate fracture behavior.<sup>25</sup>

3. Vibrational spectroscopy. The vibrational eigenstates of molecular and crystalline systems can now be calculated either via direct force-constant methods<sup>26</sup> or a linear response route,<sup>27</sup> including quantitative predictions of infrared, Raman, and inelastic neutron scattering intensities.

4. Surfaces and interfaces. Accurate calculation of surface and interface energies enables the prediction of the morphology of nanoclusters and precipitate shapes. *Ab initio* MD has made it possible to resolve even very complex surface reconstructions.<sup>28</sup>

5. Adsorption, reactions, and catalysis. Whereas theoretical studies previously have been restricted to ideal low-index surfaces, recent advances permit the investigation of molecular adsorption and reactions at stepped, kinked, and defective surfaces<sup>29</sup> and the simulation of catalytic reactions under realistic conditions of temperature and pressure. Acid-catalyzed reactions at the internal surfaces of functionalized microporous and mesoporous materials have been studied using a variety of DFT techniques.<sup>30</sup>

6. Spectroscopy and dielectric properties. The possibility of calculating the polarizability of a material via a Berry phase approach has led to a new quality of calculated optical spectra<sup>31</sup> and has opened the way toward an *ab initio* treatment of ferroelectricity<sup>32</sup> and piezoelectricity.<sup>33</sup> Tools for calculating nuclear magnetic resonance spectra<sup>34</sup> and for scanning tunneling spectroscopy<sup>35</sup> have been developed.

7. Magnetic properties. A fully relativistic treatment is required to tackle problems related to magnetic anisotropy; a vector-field treatment of magnetization density is necessary for the description of the complex

non-collinear structure of frustrated antiferromagnets where exchange interactions and lattice topology are in conflict.<sup>36</sup>

8. Electronic transport. The development of tools for the calculation of electronic transport processes in nanostructured materials is a very active field. Particular attention has been paid to transport in systems showing giant magnetoresistance<sup>37</sup> and in molecular devices.<sup>38</sup>

9. Liquids and glasses. Although diffraction experiments yield the full three-dimensional structure for crystalline materials, these techniques yield only one-dimensional projections of the structure of liquids and glasses. *Ab initio* MD leads to highly accurate structural prediction for liquids and glasses without the use of empirical force fields.<sup>39</sup>

Only a few references are given in this section for lack of space; the reader is referred to the Internet home pages of the most important *ab initio* codes (see Table I).

## Multiscale Modeling: Bridging the Gaps in Time and Length Scales

It is clear that substantial gaps exist between the dimensions of even the largest systems accessible to DFT simulations and between the maximum time span of *ab initio* MD simulations and the time and length scales of laboratory experiments. To bridge these gaps, strategies for multiscale simulations are being developed. This task is tackled from different sides. Configurational free energies of extended systems, including substitutional disorder in multicomponent systems, can be obtained from cluster-expansion methods, which extract representative lattice models from DFT that can then be used in Monte Carlo simulations to obtain such quantities as temperature–composition phase diagrams, short-range order of disordered phases, interfacial free energies, and precipitate shapes.<sup>40,41</sup> The special quasi-random structure approach<sup>42</sup> makes possible the direct calculation of electronic and energetic properties of disordered systems using small-unit-cell structures amenable to DFT. These models have been implemented with significant success and lead to true structure predictions, later verified by experiments.<sup>43</sup> In a similar spirit, DFT computations of the formation energy of intermetallic compounds have been used as input in the CALPHAD models for the thermodynamics of materials.<sup>44</sup> One new area that holds considerable promise is the integration of DFT with phase-field models to study the evolution of microstructures.<sup>45</sup> DFT can be used to compute such quantities as free energies, diffusion constants, and interfacial energies. These first-principles-predicted

quantities can then serve as the thermodynamic and kinetic driving forces for the phase-field models of microstructural evolution.

Another strategy for solving the length scale problem is embedding. For a small reactive center where atomistic resolution and high accuracy are important, a calculation at a high level of sophistication is performed. The boundary conditions for this calculation are determined by a treatment of the area surrounding the center at a lower level. Examples for this approach are the quantum-mechanical/molecular modeling approach used in heterogeneous catalysis;<sup>46</sup> the description of crack propagation using DFT to simulate the crack tip, embedded in an atomistic force-field description of the strain field at intermediate distances; and a continuum approach on a macroscopic scale. A particularly attractive version of this embedding scheme is the “learn-on-the-fly” strategy,<sup>47</sup> where local quantum computations are used to continually tune the parameters of the force field used for the classical part of the simulations.

Time-scale gaps are caused by energy barriers for chemical reactions and first-order structural phase transitions. Rare events such as activated chemical reactions can be treated within transition-state sampling methods;<sup>48</sup> temperature-accelerated MD methods<sup>49,50</sup> or metadynamic techniques.<sup>51</sup> This allows one to identify novel phases under extreme thermodynamic conditions and to trace out transformation pathways for structural phase transitions. Kinetic Monte Carlo simulations can be used to simulate growth processes or chemical reactions on regular lattices under realistic conditions of temperature.

## Hardware

DFT simulations of materials do not require supercomputer resources. A typical hardware base for such simulations consists of a PC cluster with fast processors equipped with sufficient memory ( $\geq 1$  Gbyte) and a fast interconnect. Modern DFT codes offer efficient simulation of medium-sized systems on clusters of about 32 CPUs.

## Applications of DFT in Materials Research

This issue of *MRS Bulletin* collects a diversity of DFT success stories from such wide-ranging materials research topics as surface science and catalysis, earth sciences, nanotechnology, and structural metals. Of course, any such list of examples will necessarily be incomplete, but it should give the reader a sense of the

types of capabilities and opportunities presently at hand.

## Mechanical Properties and Structural Materials

The article by Ikehata et al. from the Toyota research group of Takashi Saito describes a specific example of the use of DFT in an alloy design problem, namely, the search for a low-modulus, high-strength titanium alloy. This article provides an excellent illustration of the power of a combined theoretical and experimental approach directed toward the search for a material with specified properties.

Applications of DFT to structural materials also exist in steels, notably, the work of Olson and co-workers,<sup>52</sup> who use various computational materials techniques to accelerate the design process of new high-strength steels. The Virtual Aluminum Castings program at Ford Motor Company involves the use of DFT and its connection to higher-length-scale modeling tools<sup>44,45</sup> directed toward improved processing and enhanced properties of aluminum cast alloys.

A novel MD approach combining quantum-mechanical embedding with classical force-field models has been used by Csanyi et al.<sup>47</sup> to model crack propagation in silicon using a model containing about 200,000 atoms (see Figure 1). About 300 atoms near the crack tip are treated quantum-mechanically, and this is essential for a correct description of the  $(2 \times 1)$  periodicity of the reconstruction of the crack surface. Although this method has currently been applied to Si, future extensions of this method to structural materials could produce useful insight on crack propagation in a variety of materials types.

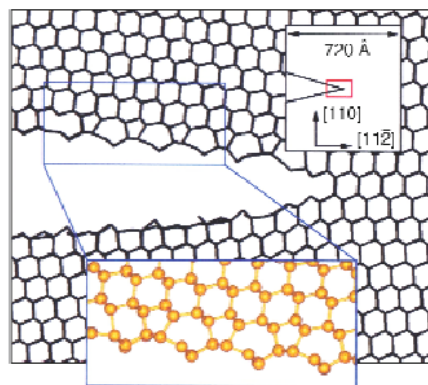


Figure 1. Propagation of a  $(111)[110]$  crack in silicon, modeled using the “learn-on-the-fly” scheme mixing quantum and classical simulations. Note the  $(2 \times 1)$  periodicity of the reconstruction appearing on the upper opening surface. After Csanyi et al.<sup>47</sup>

## Catalysis and Surface Science

Electronic-structure calculations have been used extensively in the fields of surface science and catalysis. Nørskov et al. review how DFT is being used to elucidate atomic-scale mechanisms for chemical reactions on surfaces and to quantitatively describe the rates of heterogeneous catalysis reactions. These authors also provide an intriguing discussion of the future prospects of the calculations to predict new catalysts and, hence, provide a rational guide for catalyst development. DFT techniques are also applied to the investigation of acid-based catalysis by microporous materials such as zeolites. An interesting innovation is the production of  $\epsilon$ -caprolactam (a precursor molecule to the polymer nylon-6) by conversion of cyclohexanone (the so-called Beckmann rearrangement) in a zeolite or a structurally related aluminophosphate,<sup>53,54</sup> a reaction that is environmentally much more benign than the conventional route through homogeneous catalysis in sulfuric acid. Figure 2 shows the final step in the formation of  $\epsilon$ -caprolactam, the hydrolysis of an intermediate carbiminium ion in the pore of a zeolite.

## Magnetism and Magnetic Materials

The enormous increase in the recording density of hard disk drives by eight orders of magnitude during the past 50 years (see the May 2006 issue of *MRS Bulletin* on “Materials for Magnetic Data Storage”) has been achieved by downsizing the bits recorded in the magnetic storage layer. This approach is, however, limited by the onset of superparamagnetism, which occurs when the grain size in the recording medium is reduced to an extent that the magnetic energy stored in a grain becomes comparable to the thermal energy. Recently, based on DFT calculations, tetragonal iron cobalt alloys were proposed as promising materials with the desired high uniaxial magnetic anisotropy and high saturation magnetization.<sup>55</sup> Stability of the tetragonal FeCo phase can be achieved in FeCo/Pt superlattices (see Figure 3); again, DFT calculations turned out to be essential.<sup>56</sup> This is a good example of a real computer-aided materials design.

## Oxides and Minerals

DFT works quite well on oxides of alkali, alkaline-earth, and main group elements. In their article, Brodholt and Vocollo describe the uses of DFT in geology and the earth sciences. Calculations have the ability to simulate conditions in the Earth’s interior that would otherwise be quite problematic to reproduce in the laboratory. Applications of DFT have

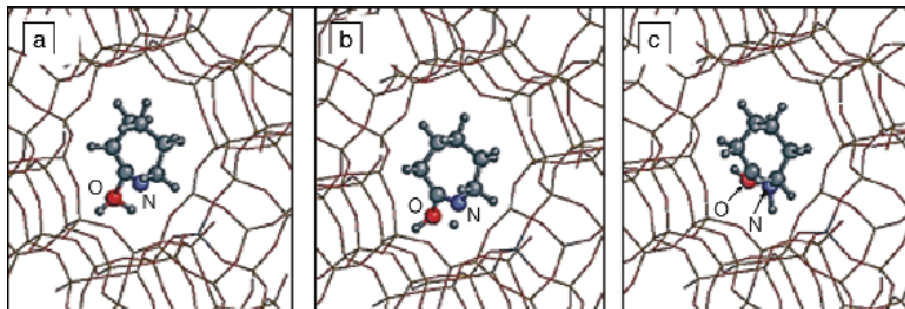


Figure 2. (a) Initial, (b) transition, and (c) final states of the hydrolysis of a carbiminium ion to form N-protonated  $\epsilon$ -caprolactam, catalyzed by an acid zeolite. After Bucko et al.<sup>54</sup>

predicted such fundamental properties as the properties of iron and (Mg,Fe)SiO<sub>3</sub> under the extreme pressures and temperatures of the Earth's interior. DFT calculations have also recently been shown to put bounds on the possible composition of the Earth's core and have identified a new phase of (Mg,Fe)SiO<sub>3</sub> just above the core. The application of DFT in transition-metal oxides requires considerably more care, as the spurious self-interaction in DFT overly delocalizes electrons, leading to excessive metallic behavior and the washing out of mixed-valence states in doped oxides, affecting local spin magnetism, conductivity, and even phase stability. Despite these limitations, DFT and enhanced DFT methods can be used to assist in the rational design of new materials. A good example can be found in the search for a

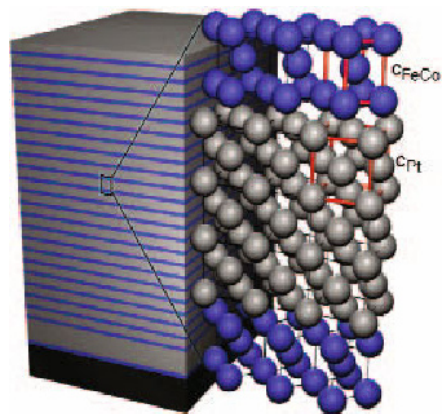


Figure 3. Schematic of the tetragonal "3/7" superlattice of an Fe<sub>0.36</sub>Co<sub>0.64</sub> alloy and Pt, showing a huge perpendicular magnetic anisotropy energy (the lattice parameters are  $C_{FeCo} = 0.317$  nm and  $C_{Pt} = 0.417$  nm). This superlattice has been proposed on the basis of DFT calculations and experimentally realized by sputter deposition. After Andersson et al.<sup>55</sup>

lithium-battery electrode material with higher energy and power density.<sup>43</sup> In this field, DFT computations are now commonplace in industry and academic labs.

### Semiconductors and Nanotechnology

Semiconductors probably form the class of materials that has seen the most widespread use of DFT. Calculations of electronic properties for known semiconductors, such as bandgaps and defect states, are now commonplace and have been performed for virtually all unary and binary semiconductor systems as well as for a wealth of higher-order compounds, ordered and disordered alloys, dopant types, and surface structures. In his contribution to this issue, Marzari reviews the applications of DFT to semiconductor nanotechnology, concentrating on Si-H nanostructures, single-walled carbon nanotubes, and self-assembled monolayers. The combined investigation, based on experiment and DFT calculations, of the adsorption of large organic molecules on metallic and semiconducting surfaces, the formation of ordered structures through a self-assembly process,<sup>57</sup> and the electronic transport process in these molecular devices<sup>58</sup> is an essential contribution toward the development of molecular electronics.

### Biomaterials

DFT calculations play an increasingly important role for understanding complex processes in biological materials. For example, the protonation of the retinal chromophore is of crucial importance for the visual process. Protonation leads to the formation of a highly polarizable  $\pi$ -system required for long-wavelength adsorbance and wavelength regulation by the protein environment, and deprotonation is required for the protein to reach the activating state after light adsorption. Sugihara et al.<sup>58</sup> and Röhrig et al.<sup>59</sup> have applied DFT techniques to investigate the structure

and dynamics of the retinal chromophore of rhodopsin in different environments. Figure 4 shows the DFT-optimized structure of the chromophore binding site. One of the exploratory studies based on a linear-scaling code presents a total energy calculation of a piece of DNA consisting of more than 2500 atoms.<sup>17</sup>

### High-Throughput Ab Initio Calculations

High-throughput (combinatorial) experimentation has played an increasingly important role in materials science. By studying large numbers of systems, one can screen combinatorial spaces for new systems with desired properties. Modern DFT codes have now become very robust, enabling many tasks to be performed automatically. Combined with the increasing speed of computers, this opens the way toward high-throughput computation.<sup>60</sup> Pioneering applications have been devoted to crystal structure predictions<sup>61</sup> and the search for stable quaternary alloys.<sup>62</sup>

### Summary and Outlook

DFT is the most detailed "microscope" currently available to glance into the atomic and electronic details of matter. As such, it has catalyzed a renewed interest into the fundamental science, chemistry, and physics of materials. Its impact is likely to continue to grow through the further development of tools that build upon DFT to model higher-level properties not directly accessible to DFT because of time-scale, length-scale, or complexity issues. Much of this application-driven modeling is likely to be performed by people with field-specific knowledge in cooperation with the DFT practitioners and code developers; therefore, educating the materials

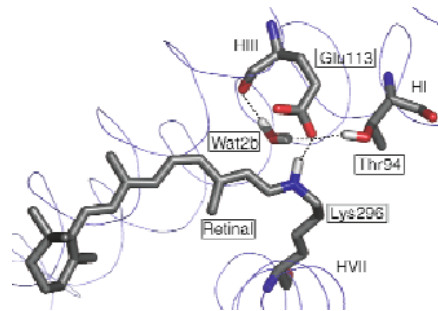


Figure 4. Schematic of the DFT energy-optimized structure of the chromophore binding site in rhodopsin of a protonated 11-cis-retinal Schiff base (Lys296) in contact with a glutamate ion (Glu113), an amino acid (Thr94), and a water molecule (Wat2b). HI, HIII, and HVII are regions in mitochondrial DNA. After Sugihara et al.<sup>58</sup>

scientists of the future through new textbooks, online courses, and tutorials is a crucial aspect of increasing the impact of DFT.

Despite all of its successes, DFT is not accurate for all problems. We have already mentioned the continuing effort to construct exchange-correlation functionals leading to improved accuracy. Although DFT does an excellent job on the ground-state properties of metals and semiconductors, the “bandgap” problem (i.e., the difficulty of achieving a quantitatively accurate prediction of the gap between the highest occupied and the lowest empty eigenstates) and the inability to describe the physics of van der Waals interactions are notorious. Also, the properties of strongly correlated systems such as transition-metal oxides are not well reproduced by common exchange-correlation functionals. Evidently, explorations of the many-body aspects of electron correlation beyond current DFT methods are needed, and this is currently a very active field of research. Many-body perturbation theory (the GW method) corrects most of the bandgap problem in DFT, even for difficult cases such as narrow-gap semiconductors.<sup>63</sup> LDA+*U* approaches combine a DFT description of extended states with a Hartree-Fock-like treatment of the Coulomb repulsion *U* between states in narrow *d*- and *f*-bands, and lead to a significant improvement in the structural, electronic, magnetic, and optical properties of transition-metal oxides<sup>64</sup> and other systems where electron localization is strong. Dynamic mean-field theory (DMFT) may be considered as a many-body extension of DFT that attempts to capture the true many-body physics of the electron-electron interaction. For strongly correlated systems, LDA+DMFT agrees with LDA+*U*, but it subsumes the LDA for weakly correlated metals and achieves a correct description of arbitrary strength of the onsite Coulomb repulsion.<sup>65</sup> At this point, no unified “post-DFT” theory exists, and practitioners will need to decide with care which improvement strategy is best suited for a property that cannot be accurately computed at the DFT level. Finally, the recent development of a highly efficient quantum Monte Carlo approach<sup>66</sup> could open the way toward materials simulations with an unprecedented level of accuracy and sophistication.

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**Jürgen Hafner**

**Jürgen Hafner**, Guest Editor for this issue of *MRS Bulletin*, is a professor of Solid-State Sciences at the University of Vienna and director of the Graduate College for Computational Materials Science. He graduated in 1973 from Vienna Technical University, where he also was appointed professor of theoretical physics in 1982 after serving for several years as a research associate at the Max Planck Institute for Solid-State Sciences. In 1998, he accepted a chair at the Faculty of Physics of the University of Vienna.

Hafner's research concentrates on the application of density functional methods to a wide range of problems in materials science, from magnetism at the nanoscale to surface science and catalysis. He has received the Ludwig Boltzmann Prize from the Austrian Physical Society and the Erwin Schrödinger Award of the Austrian Academy of Sciences. Also, Hafner has authored more than 500 publications in refereed international journals.

Hafner can be reached at Universität Wien, Institut für Materialphysik and Center for Computational



**Christopher Wolverton**

Materials Science, Sensengasse 8/12, A-1090 Wien, Austria; tel. 43-4277-51400 (direct) and 43-4277-51401 (secretary), fax 43-4277-9514, and e-mail [juergen.hafner@univie.ac.at](mailto:juergen.hafner@univie.ac.at).

**Christopher Wolverton**, Guest Editor for this issue of *MRS Bulletin*, is a technical leader at Ford Research and Innovation Center, where he leads the Hydrogen Storage and Nanoscale Modeling Group. He received his PhD degree in physics from the University of California at Berkeley. After completing his PhD degree, Wolverton performed postdoctoral work at the National Renewable Energy Laboratory (NREL).

His research interests include computational studies of a variety of automotive and environmentally friendly materials via first-principles atomistic calculations and methodologies for linking atomistic and microstructural scales. Current topics of interest include the discovery of novel hydrogen storage reactions, phase transformations in metallic and oxide alloys, microstructural evolution during heat treatment, and the theoretical prediction of new materials. Wolverton



**Gerbrand Ceder**

has co-authored more than 60 peer-reviewed publications and holds two patents, with several others pending.

Wolverton can be reached at Ford Motor Company, MD 3083/SRL, PO Box 2053, Dearborn, MI 48121, USA; tel. 313-390-9552, fax 313-323-1129, and e-mail [cwolvert@ford.com](mailto:cwolvert@ford.com).

**Gerbrand Ceder**, Guest Editor for this issue of *MRS Bulletin*, is the R.P. Simmons Professor of Materials Science and Engineering at the Massachusetts Institute of Technology. He holds an engineering degree from the University of Leuven, Belgium, and a PhD degree in materials science from the University of California at Berkeley.

Ceder's research interests include first-principles predictions of materials properties and structure, with a focus on materials for energy generation and storage. He has received the Battery Research Award from the Electrochemical Society, the Career Award from the National Science Foundation, and the Robert Lansing Hardy Award from TMS.

Ceder can be reached at the Department of Materials Science and Engineering, Massachusetts



**John P. Brodholt**

Institute of Technology, Room 13-5056, 77 Massachusetts Ave., Cambridge, MA 02139, USA; tel. 617-253-1581, fax 617-258-6534, and e-mail [gceder@mit.edu](mailto:gceder@mit.edu).

**John P. Brodholt** is a professor of mineral physics in the Department of Earth Sciences at University College London. The focus of his research is computational mineral physics applied to the Earth's interior. Brodholt was awarded the European Mineralogical Union Medal for Research Excellence in 2002 and was elected as a fellow of the Mineralogical Society of America in 2005. He has published more than 90 papers in his field.

Brodholt can be reached at University College London, Department of Earth Sciences, Gower Street, London, WC1E 6BT, United Kingdom; tel. 44-0-20-7679-2622, fax 44-0-20-7388-7614, and e-mail [j.brodholt@ucl.ac.uk](mailto:j.brodholt@ucl.ac.uk).

**Hideaki Ikehata** is a researcher in the Toyota Central R&D Labs Inc. (TCRDL). He received his MS degree from Kyoto University and subsequently joined TCRDL in 1998. His research interests include strengthening of



**Hideaki Ikehata**



**Matthias Scheffler**

metallic materials and theoretical predictions of the physical properties of metals by first-principles calculations.

Ikehata can be reached at Toyota Central R&D Labs Inc., 41-1 Yokomichi, Nagakute, Aichi 480-1192, Japan; tel. 81-561-63-4660, fax 81-561-63-6156, and e-mail [ikehata@mosk.tytlabs.co.jp](mailto:ikehata@mosk.tytlabs.co.jp).

**Shigeru Kuramoto** is a researcher in the Toyota Central R&D Labs Inc. (TCRDL). He received a DEng degree from the University of Tokyo (UT) in 1994, focusing on deformation and fracture of aluminum alloys at low temperatures. Prior to joining TCRDL in 2002, Kuramoto worked as a researcher in Furukawa Electric Co. Ltd. and as a research associate at UT. His research interests are deformation and fracture in metallic materials.





**Shigeru Kuramoto**



**Nicola Marzari**



**Naoyuki Nagasako**



**Jens K. Nørskov**



**Takashi Saito**



**Hervé Toulhoat**



**Lidunka Vočadlo**

Kuramoto can be reached at Toyota Central R&D Labs Inc., 41-1 Yokomichi, Nagakute, Aichi 480-1192, Japan; tel. 81-561-63-4660, fax 81-561-63-6156, and e-mail kuramoto@mosk.tytlabs.co.jp.

**Nicola Marzari** is associate professor of computational materials science in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology. He holds a *Laurea* degree in physics from the University of Trieste in Italy and a PhD degree in physics from the University of Cambridge. Before joining MIT, he was an NSF postdoctoral fellow at Rutgers University and a research scientist with the Naval Research Laboratory and with Princeton University.

Marzari's research is dedicated to the development and application

of novel electronic-structure approaches to characterize and design advanced materials and devices. In 2005, he was the subject editor for electronic structure in the *Handbook of Materials Modeling* (Springer).

Marzari can be reached at the Massachusetts Institute of Technology, Department of Materials Science and Engineering, Room 13-5066, 77 Massachusetts Ave., Cambridge, MA 02139-4307, USA; tel. 617-452-2758, fax 617-258-6534, and e-mail marzari@mit.edu.

**Naoyuki Nagasako** is a researcher in the Toyota Central R&D Labs Inc. (TCRDL). He joined TCRDL after his receiving his MS degree from Hiroshima University in 1997. His research interests include theoretical studies on the physical properties of materials by first-principles calculations and their

application to materials design.

Nagasako can be reached at Toyota Central R&D Labs Inc., 41-1 Yokomichi, Nagakute, Aichi 480-1192, Japan; tel. 81-561-63-4537, fax 81-561-63-5426, and e-mail nagasako@mosk.tytlabs.co.jp.

**Jens K. Nørskov** is a professor of physics in the Department of Physics at the Technical University of Denmark (DTU). Also, he is director of the Center for Atomic-Scale Materials Physics, the director of NanoDTU, and the chair of the Danish Center for Scientific Computing. Nørskov received his PhD degree in physics in 1979 from the University of Aarhus in Denmark. Before his appointment at DTU in 1987, he held research positions at the University of Aarhus, IBM in Yorktown Heights, the Nordic Institute for Theoretical Physics in Copenhagen, and Halldor Topsoe. In 1993, he co-founded DTU's Center for Atomic-Scale Materials Physics.

Nørskov's research interests include theoretical surface physics, heterogeneous catalysis, nanostructures and materials properties, biomolecules, electrochemistry, and hydrogen storage. He is a

member of the Royal Danish Academy of Science and Letters, and his recent honors include the 2005 Innovation Prize from DTU and an honorary doctorate from the Technical University of Eindhoven in 2006.

Nørskov can be reached at CAMP, Department of Physics, B. 307, Technical University of Denmark, DK-2800 Lyngby, Denmark; tel. 45-4525-3175, fax 45-4593-2399, and e-mail nørskov@fysik.dtu.dk.

**Takashi Saito** is a director at the Toyota Central R&D Labs Inc. (TCRDL). He earned a DEng degree from Tohoku University in 1979, focusing on the calculation of phase diagrams and phase transformations. After receiving his degree, he joined TCRDL in 1980.

His research interests include mechanical and physical properties of high-performance metallic materials.

Saito can be reached at Toyota Central R&D Labs Inc., 41-1 Yokomichi, Nagakute, Aichi 480-1192, Japan; tel. 81-561-63-3090, fax 81-561-63-5441, and e-mail saito@mosk.tytlabs.co.jp.

**Matthias Scheffler** has been director of the Fritz

Haber Institute of the Max Planck Society in Berlin since 1988, and a Distinguished Visiting Professor at the University of California in Santa Barbara since 2005. His research areas include *ab initio* theories of electronic structure, in particular, density functional theory, quantum Monte Carlo and self-energy methods, atomistic thermodynamics, and statistical mechanics. Various hybrid methods have been developed that allow the study of mesoscopic systems and time scales from picoseconds to seconds. Also, Scheffler has investigated semiconductors, metals, transition-metal oxides, carbon nanostructures, transition-metal clusters, and biomolecules.

He was named a fellow of the American Physical Society in 1998 and was honored with the Medard W. Welch Medal and Prize in 2003 and the Max Born Medal and Prize in 2004.

Scheffler can be reached at Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany; tel. 49-30-8413-4711 and fax 49-30-8413-4701.

**Hervé Toulhoat** is deputy scientific director of the Institut Français du Pétrole (IFP) and the director of doctoral studies at IFP School in Rueil-Malmaison, France. He earned a PhD degree in chemical engineering from the Paris School of Mines in 1980, and an MSc degree from Ecole Nationale Supérieure de

Chimie de Paris in 1976. Toulhoat is a member of the Editorial Board of the *Journal of Catalysis* and an associate member of the IUPAP Commission on Computational Physics. He has authored more than 100 papers and holds 20 patents, mostly dealing with catalysis and processes in oil refining.

Toulhoat can be reached at Institut Français du Pétrole, 1-4 avenue de Bois-Préau, 92852 Rueil-Malmaison Cedex, France; tel. 33-1-47-52-73-50, fax 33-1-47-52-70-22, and e-mail [herve.toulhoat@ifp.fr](mailto:herve.toulhoat@ifp.fr).

**Lidunka Vočadlo** is a Royal Society University Research Fellow and

reader in mineral physics in the Department of Earth Sciences at University College London.

Her research interests include the Earth's core and planetary ices. She was awarded the Doornbos Prize for Research Excellence in 1998 and the 2004 Max Hey Medal of the Mineralogical Society of

Great Britain and Ireland.

Vočadlo can be reached at University College London, Department of Earth Sciences, Gower Street, London, WC1E 6BT, United Kingdom; tel. 44-20-7679-7919, fax 44-20-7679-2685, and e-mail [l.vocadlo@ucl.ac.uk](mailto:l.vocadlo@ucl.ac.uk). □

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