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# **MULTISCALE MATERIALS MODELLING PROGRAMS**

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# ABSTRACT

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## ABBREVIATIONS

ASE	Atomic Simulation Environment
BCC	Body-Centered Cubic
CC	Coupled-Cluster
COHP	Crystal Orbital Hamilton Population
CPA	Coherent Potential Approximation
CPU	Central Processing Unit
DFT	Density Functional Theory
EAM	Embedded-Atom Method
EFG	Electric Field Gradient
ELF	Electron Localization Functions
EMTO	Exact Muffin-Tin Orbitals
FCC	Face-Centered Cubic
FCD	Full Charge Density
FEM	Finite-Element Method
FFT	Fast Fourier Transform
GGA	Generalized-Gradient Approximation
GPL	General Public License
GTF	Gaussian-Type Functions
GUI	Graphical User Interface
HCP	Hexagonal Closest Packed
HF	Hartree-Fock
KS	Kohn-Sham
LBM	Lattice-Boltzmann Method

LCGTO	Linear Combination of Gaussian-Type Orbital
LDA	Local Density Approximation
LEED	Low Energy Electron Diffraction
MBPT	Many-Body Perturbation Theory
MC	Monte Carlo
MD	Molecular Dynamics
MM	Molecular Mechanics
MPI	Message Passing Interface
OEP	Optimized Effective Potential
PAW	Projector-Augmented Wave
SCC	Self-Consistent Charge
SCF	Self-Consistent Field
TB	Tight Binding
TDDFT	Time-Dependent Density Functional Theory
QMC	Quantum Monte Carlo

# 1 INTRODUCTION

The main goal of this study is to gather a database of multiscale modelling programs. A demand of gathered information about available programs have arisen and therefore this database is done. There is a great amount of these programs available, but as it is they are time consuming to find and interpret. The programs are searched especially known to be used within the European cooperation in science and technology (COST) Action P19. During the search also other interesting programs are found and some of them are added to database also. Furthermore it is clear that there is available a great amount of multiscale modelling codes, but it is not possible to introduce all of those within the limits of this study.

Also some calculation is done using one particular code: Aimpro. These calculations are secondary of importance for this work and are not to be complete at this time. Nevertheless through those a better perspective to the main goal of the study is achieved. Worth mentioning is nevertheless that the calculations are about the movement of lithium within graphite layers.

# 2 ABOUT MULTISCALE MATERIALS MODELLING

The discovery and development of materials was, for a long time, subject of chance and empirical trial and error methods. This situation has dramatically changed. Nowadays the structure-property relations are well-known and so the properties of materials can be predicted on the basis of their structure. [1]

Multiscale modelling is an emerging topic in material properties field, because the structure of materials on microscopic level controls their macroscopic properties. Multiscale modelling is needed to link different time and length regions as illustrated in figure 1. The increasing computer power makes it possible to perform calculations of atomic structure in large extent and create the basis for understanding and employing the structure-property relation. European research groups have been in the front-line in development of new multiscale modelling methods. [1]



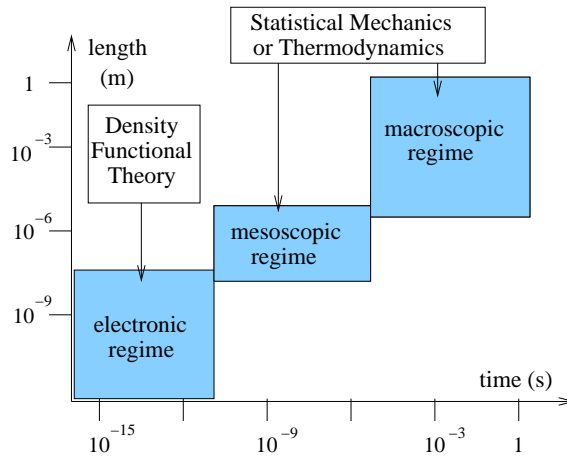


Figure 1: Multiscale material modelling

## 2.1 CLASSIFICATION OF PROGRAMS

As stated earlier a great amount of different kinds of multiscale modelling programs can be found only by searching the internet a cut of these is listed in this study. However there is 55 programs introduced here. The programs could be classified in different ways and sometimes they overlap classifications by their features. However to make the database user-friendly the following classification of multiscale modelling programs is made: Ab initio; Tight binding; Classical molecular dynamics; Classical Monte carlo; Micromagnetism; Lattice-Boltzmann and Finite-element method; Other methods. Within these groups there is mentioned in case the particular program is commercial or non commercial. Of course mainly the database is about non commercial programs, but there are few exceptions. Some of the non commercial programs involve a license or a small fee in order to use the program. These programs are however classified as non commercial by taking into account their nature of development and distribution.

Consequently to the amount of available multiscale modelling programs nowadays: There is amount of programs, that come up during the search for the database, but nevertheless could not been added to it. These programs are however mentioned in the very end of the section database.

### **2.1.1 AB INITIO**

The Latin term *ab initio* means from the beginning. Here by the term *ab initio* is referred to electronic structure methods. There are two main techniques, wave-function and electron-density based methods that originate from quantum chemistry and solid-state physics [2]. The *ab initio* methods are computationally heavy and expensive.

### **2.1.2 TIGHT BINDING**

Total energy calculations are computationally rather expensive. There is a computational scheme of the early days of computational physics that is still rather popular: the tight-binding method in which the essentials of quantum mechanics are retained. In short, the tight-binding method can be characterized by saying that it assumes an expansion of the eigenstates of the effective one-particle Hamiltonian in an atomic-like basis set and replaces the exact many-body Hamiltonian with parametrized Hamiltonian matrix elements. A tight-binding method in parametrization of *ab initio* potentials is more time consuming than an analytical representation since it requires the diagonalization of a matrix. However, due to the fact that the quantum mechanical nature of bonding is taken into account, tight-binding schemes need a smaller number of *ab initio* input points to perform a good interpolation and extrapolation. [2]

### **2.1.3 CLASSICAL MOLECULAR DYNAMICS AND MONTE CARLO**

Molecular simulations is a generic term encompassing both Monte Carlo (MC) and molecular dynamics (MD) computing methods. The feature that distinguishes molecular simulation from other computing methods and approximations is that the molecular coordinates of the system are evolved in accordance with a rigorous calculation of intermolecular energies and forces. Molecular simulation can be aptly described as computational statistical mechanics. Molecular simulation determines the individual forces experienced by each molecule. Molecular modelling is a contrast to electronic structure calculations where electrons are considered explicitly. The benefit is obviously that it reduces the complexity of the system. Calculating the interaction between molecules is at the heart of either a Monte Carlo or molecular dynamics simulation program. The Monte Carlo method is a stochastic strategy that relies on probabilities. In contrast to the Monte Carlo method which relies on transition probabilities, molecular dynamics solves

the equations of motion of the molecules to generate new configurations. Consequently, MD simulations can be used to obtain time-dependent properties of the system. [3]

#### **2.1.4 OTHER METHODS**

Programs for micromagnetic simulations are classified separately from others. Also Lattice-Boltzmann method (LBM) and finite element method programs are in a separate group, for their different nature from preceding programs. The finite element method is used with applications of solid mechanics; fluid mechanics; heat, mass and energy transfer, etc. The Lattice-Boltzmann method has emerged more recently with intensive application to thermal-fluid problems. [4]

#### **2.1.5 REST OF THE PROGRAMS**

After all of the preceding methods mentioned there is still some more programs listed that do not belong into any of the preceding groups. For example the program Symmetrized Automated Tensor Low Energy Electron Diffraction (SATLEED) bases on comparison of experimental and calculated Low Energy Electron Diffraction I/V-spectra. [5]

### **3 DATABASE**

All the programs are listed in this main section named database. For each program the following information can be found: availability, main features of program, development of program and for the most a webpage, where further information can be found. The programs are listed in groups: Ab initio; Tight binding; Classical molecular dynamics and monte carlo; other methods; and programs used in interpretation of experimental data. Within these groups the non commercial programs are listed first and after those are the commercial programs, both in alphabetical order. This feature is stated in the beginning of each object, in the availability paragraph.

## 3.1 AB INITIO PROGRAMS

### 3.1.1 ABINIT

Main characteristic: Ab initio.

Availability: Non commercial. Starting from version 3, ABINIT is distributed under the GNU General Public License.

Introduction: ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a planewave basis. ABINIT also includes options to optimize the geometry according to the DFT forces and stresses, or to perform molecular dynamics simulations using these forces, or to generate dynamical matrices, Born effective charges, and dielectric tensors. Excited states can be computed within the Time-Dependent Density Functional Theory (for molecules), or within Many-Body Perturbation Theory (the GW approximation). The sequential version of the main code is named abinis (ABINIT sequential) and the parallel version is named abinip (ABINIT parallel). [6] ABINIT calculator is compatible with the Atomic Simulation Environment (ASE). ASE is written in the programming language Python with the aim of setting up, steering and analyzing atomistic simulations. [7]

Further info: <http://www.abinit.org/>.

Development: Since the beginning of the project, in 1997, several groups have shown a clear commitment to the ABINIT project:

- J.-M. Beuken, X. Gonze, G.-M. Rignanese, L. Sindic ... (Université Catholique de Louvain, Belgium)
- G. Zerah, F. Jollet, M. Torrent, G. Jomard, A. Roy, V. Recoules... (Commissariat Energie Atomique, Bruyeres, France)
- M. Mikami (Mitsubishi Chemical Corp., Japan)
- Ph. Ghosez, J.-Y. Raty (Université de Liege, Belgium)
- L. Reining, V. Olevano, G. Onida, R. Godby (contributors to the GW part of ABINIT, from Ecole Polytechnique Palaiseau (France), U. Roma (Italy), U. of York (UK), U. Grenoble)
- D. Vanderbilt, D. Hamann (Rutgers U., USA)
- M. Coté (U. de Montréal, Canada)

[8]

### 3.1.2 ACES II

Main characteristic: Ab initio.

Availability: Non commercial. License, free of charge?

Introduction: ACES II is a set of programs that perform ab initio quantum chemistry calculations. The package is highly flexible and supports many kinds of calculations at a number of levels of theory. The major strength of the program system is using "many-body" methods to treat electron correlation. These approaches, broadly categorized as many-body perturbation theory (MBPT) and the coupled-cluster (CC) approximation, offer a reliable treatment of correlation and have the attractive property of size-extensivity, which means that the energies scale properly with the size of the system. As a result of this property, MBPT and CC methods are ideally suited for the study of chemical reactions. Although the ACES II can perform Hartree-Fock Self-Consistent-Field (HF-SCF) and Kohn-Sham Density Functional Theory (KS-DFT) calculations, it is not intended for large scale HF-SCF or KS-DFT calculations. [9]

Two important features of the ACES II program system are its effective use of molecular symmetry, particularly in MBPT and CC calculations, and the sophisticated gradient methods which are included in the program. [9]

Further info: <http://www.qtp.ufl.edu/Aces2/>

and a manual: <http://www.qtp.ufl.edu/Aces2/man-aces2.pdf>.

Development: ACES II is a program product of the Quantum Theory Project, University of Florida. Authors: J.F. Stanton, J. Gauss, S.A. Perera, J.D. Watts, A.D. Yau, M. Nooijen, N. Oliphant, P.G. Szalay, W.J. Lauderdale, S.R. Gwaltney, S. Beck, A. Balkova, D.E. Bernholdt, K.K. Baeck, P. Rozyczko, H. Sekino, C. Huber, J. Pittner, W. Cencek, D. Taylor, and R.J. Bartlett. Integral packages included are VMOL (J. Almlöf and P.R. Taylor); VPROPS (P. Taylor); ABA-CUS (T. Helgaker, H.J. Aa. Jensen, P. Jørgensen, J. Olsen, and P.R. Taylor); HONDO/GAMESS (M.W. Schmidt, K.K. Baldrige, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.J. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S. Su, T.L. Windus, M. Dupuis, J.A. Montgomery). [9]

### 3.1.3 AIMPRO

Main characteristic: Ab initio.

Availability: Non commercial. License, free of charge?

Introduction: Aimpro is an electronic-structure program using Local Density Approximation (LDA)- and Generalized-Gradient Approximation-Density Functional Theory (GGA-DFT). Atoms are treated using pseudopotentials to remove the core electrons, and the distribution of the electrons solved self-consistently for a given set of atoms. In addition to the efficiencies offered by their separability, the latter pseudopotentials offer extended norm conservation, accounting for a large number of occupied and unoccupied atomic levels. AIMPRO uses, by default, the Perdew-Wang functional for PBC calculations and a Padé approximation to this functional for cluster calculations, although a number of alternative functionals are available. GGA calculations are performed using a White-Bird implementation of the GGA functional. Aimpro can be used with a range of pseudopotential types, including the seminonlocal forms, and the dual-space separable pseudopotentials. [10] The newest version of Aimpro is v2.1.4. [11]

AIMPRO can be used both in periodic and cluster modes and the atomic structures optimized either using static minimization methods or molecular dynamics. A range of observables can be derived from these calculations, such as the electrical levels, vibrational-mode frequencies and symmetries, electronic-structures, hyperfine and zero-field splitting tensors, electron energy loss spectra, migration barriers, and so on. However, in contrast to the majority of PBC calculations, AIMPRO represents the wave-functions using a range of real-space, Gaussian-orbital functions. [10]

Further info: <http://aimpro.ncl.ac.uk/>

Development: Patrick Briddon.

### 3.1.4 CPMD

Main characteristic: Ab initio.

Availability: Non commercial. Distributed free of charge to non-profit organizations.

Introduction: The CPMD code is a parallelized plane wave/pseudopotential implementation of Density Functional Theory. It is designed particularly for ab-initio molecular dynamics. Current version is 3.13. [12]

CPMD main characteristics:

- works with norm conserving or ultrasoft pseudopotentials
- LDA, LSD and the most popular gradient correction schemes; free energy density functional implementation

- isolated systems and system with periodic boundary conditions; k-points
  - molecular and crystal symmetry
  - wavefunction optimization: direct minimization and diagonalization
  - geometry optimization: local optimization and simulated annealing
  - molecular dynamics: constant energy, constant temperature and constant pressure
  - path integral MD
  - response functions
  - excited states
  - many electronic properties
  - time-dependent DFT (excitations, molecular dynamics in excited states)
  - coarse-grained non-Markovian metadynamics
- [12]

CPMD is copyrighted jointly by IBM Corp and by Max Planck Institute, Stuttgart, and is distributed free of charge to non-profit organizations. [12]

Further info: <http://www.cpmid.org/>.

Development: During the years many people from diverse organizations contributed to the development of the code and of its pseudopotential library: Michele Parrinello, Jurg Hutter, D. Marx, P. Focher, M. Tuckerman, W. Andreoni, A. Curioni, E. Fois, U. Roetlisberger, P. Giannozzi, T. Deutsch, A. Alavi, D. Sebastiani, A. Laio, J. VandeVondele, A. Seitsonen, S. Billeter and others. [12]

### 3.1.5 DACAPO

Main characteristic: Ab initio.

Availability: Non commercial. Free of charge.

Introduction: Dacapo is a total energy program based on density functional theory. It uses a planewave basis for the valence electronic states and the core-electrons are described with Vanderbilt ultrasoft pseudo-potentials. The program performs self-consistent calculations for both Local Density Approximation (LDA) and various Generalized Gradient Approximation (GGA) exchange-correlations potentials, using state-of-art iterative algorithms. The code can perform molecular dynamics/structural relaxation simultaneous with solving the Schrödinger equations within DFT. The program may be compiled for serial as well as parallel execution. The current version is controlled externally from

ASE. [13] ASE is written in the programming language Python with the aim of setting up, steering and analyzing atomistic simulations. [7]

Further info: <http://dcwww.camd.dtu.dk/campos/Dacapo/>  
and <https://wiki.fysik.dtu.dk/dacapo/Dacapo>.

### 3.1.6 DEMON2K

Main characteristic: Ab initio.

Availability: Non commercial. The academic license of DeMon2k is free of charge.

Introduction: DeMon (density of Montréal) is a software package for density functional theory (DFT) calculations. It uses linear combination of Gaussian-type orbital (LCGTO) approach for the self-consistent solution of the Kohn-Sham (KS) DFT equations. The calculation of the four-center electron repulsion integrals is avoided by introducing an auxiliary function basis for the variational fitting of the Coulomb potential. List of main features of the package:

- Variational fitting of the Coulomb potential
- Geometry optimization and transition state search
- Molecular dynamic simulations (MD)
- Time-dependent DFT (TD-DFT)
- Calculation of properties like polarizabilities, hyperpolarizabilities, NMR, IR and Raman spectra and intensities, thermodynamic data
- Parallelized code Message Passing Interface (MPI)

[14]

Further info: [http://demon-software.com/public\\_html/program.html](http://demon-software.com/public_html/program.html).

Development: The first available version of deMon appeared in 1992. The AllChem project started in Hannover in 1995 independently of the deMon project. First AllChem version appeared in 1997. The deMon and AllChem developers agreed at the first deMon Developers meeting in Ottawa to merge their codes in order to keep a Tower of Babel from arising. The merged code was presented for the first time at the third deMon Developers meeting in Geneva. The present version of the code is now known as deMon2k to distinguish it from the earlier (premerge) codes. [14]



### 3.1.7 EMTO PROGRAM PACKAGE

Main characteristic: Ab initio.

Availability: Non commercial. The full EMTO program package can be obtained upon request from Levente Vitos: Levente.Vitos@fysik.uu.se [15].

Introduction: Exact Muffin-Tin Orbitals (EMTO) method. Despite the developments during the last few decades, an accurate ab initio description of substitutional random alloys seemed unreachable. However, along the development of the EMTO method, a distinct step was made towards the modern computational alloy theory by merging the most efficient theories of random alloys with advanced density functional techniques. The implementation and application of the EMTO theory combined with the Coherent Potential Approximation (EMTO-CPA) and the Full Charge Density (FCD) technique is the focus of the present work. The Kohn-Sham method created on this platform is referred to as the EMTO method. The most important and prominent feature of the EMTO method is that this approach is suitable for the determination of the energy changes due to anisotropic lattice distortions in ordered systems, in alloys with chemical disorder as well as in alloys with both chemical and magnetic disorder. [15]

Further info: Levente Vitos, Computational quantum mechanics for materials engineers -The EMTO method and applications. Springer-Verlag London Limited (2007). Also directly from Levente Vitos: Levente.Vitos@fysik.uu.se.

### 3.1.8 FLEUR

Main characteristic: Ab initio.

Availability: Non commercial. Freely available.

Introduction: FLEUR is a feature-full FLAPW (full potential linearized augmented plane wave) code, based on DFT. The FLAPW-Method (Full Potential Linearized Augmented Plane Wave Method) is an all-electron method which within density functional theory is universally applicable to all atoms of the periodic table and to systems with compact as well as open structures. It is very precise electronic structure method in solid state physics. Due to the all-electron nature of the method, partially occupied f-states in Lanthanides can be treated, magnetism is included rigorously and nuclear quantities e.g. isomer shift, hyperfine field, electric field gradient (EFG), and core level shift are

calculated routinely. Also open systems such as surfaces, deposited and free wires and chains, tubular systems, clusters or inorganic molecules represent no basic problem. The capability of calculating the forces exerted on the atoms within the LAPW method opens the gate to structure optimization and molecular dynamics and puts this method up on the same category as the widespread pseudopotential method, but is able to treat systems unattainable by the pseudopotential method. [16]

Features in detail:

- Bulk, film and wire geometry. FLEUR can use a truly two-dimensional basis-set or one dimensional basis-set and can thus calculate ultra-thin films or wires, without the need of supercell setups.
- More than one energy panel
- Local orbitals to supplement the LAPW-basis.
- Forces exerted on the atoms
- Electric fields applied to surfaces.
- Spin-Orbit interaction in combination with magnetism.
- Non-collinear magnetic structures with and without external constraints, spiral spin density waves.
- Full-relativistic treatment of core electrons (Dirac + Magnetism).
- LDA XC:  $X-\alpha$ , Wigner, MJW, VWN, Perdew-Zunger, BH; GGA XC: PW91, PBE.
- LDA+U
- Quasi-Newton-Methods to accelerate charge self-consistency.
- Massive parallelization: Both the k-point loop and the eigenvalue-problem are parallelized and scale very well on MPI machines.

[16]

Further info: <http://www.flapw.de/pm/index.php>.

Development: A lot of people contributed to the code. The main work is done within the group in Juelich. Current group members: Stefan Blügel, Gustav Bihlmayer, Daniel Wortmann, Christoph Friedrich, Marcus Heide, Marjana Lezaic, Manfred Niesert, Frank Freimuth, Markus Betzinger. Former group members: Arno Schindlmayr, Jussi Enko-vaara, Yuri Mokrousov, Stefan Heinze, Philipp Kurz, Xiliang Nie, Friedrich Foerster, Sean Clarke, Robert Abt, Alexander Shick, Rossitza Pentcheva. [16]

### 3.1.9 GPAW

Main characteristic: Ab initio.

Availability: Non commercial. GPAW is released under the GNU Public License version 2.

Introduction: GPAW, Grid-based Projector-Augmented Wave method, is a density functional theory code and bases on the projector-augmented wave (PAW) method. It uses real-space uniform grids and multigrid methods or atom-centered basis-functions. Using the PAW method allows one to get rid of the core electrons and work with soft pseudo valence wave functions. The pseudo wave functions don't need to be normalized - this is important for the efficiency of calculations involving 2. row elements and transition metals. A further advantage of the PAW method is that it is an all-electron method (frozen core approximation) and there is a one to one transformation between the pseudo and all-electron quantities. GPAW is written in the programming language Python. The code has been designed to work together with the atomic simulation environment (ASE). [17]

ASE is written in the programming language Python with the aim of setting up, steering and analyzing atomistic simulations. [7]

Further info: <https://wiki.fysik.dtu.dk/gpaw/index.html>.

Development: J. J. Mortensen, L. B. Hansen, and K. W. Jacobsen. Further GPAW development can be done by anyone.

### 3.1.10 LMTART

Main characteristic: Linear-muffin-tin-orbital. Tight binding.

Availability: Non commercial. LmtART is a free scientific software.

Introduction: LmtART - a Full Potential LMTO Program. The program LmtART is an implementation of full-potential linear-muffin-tin-orbital method for electronic-structure calculations. It is designed to perform band structure, total energy and force calculations within the methods of density functional theory (DFT). [18]

New version, LmtART 6.50, is now available. Its main features include:

- Local (spin) density approximation (LSDA) is available in many parametrizations to-

gether with the gradient corrected density functionals (GGA91 and GGA96).

- Multiple-kappa LMTO basis sets and multi-panel technique.
- Total energy and force calculations for determining the equilibrium structure and phonons.
- LDA+U method for strongly correlated systems.
- Spin-orbit coupling for heavy elements.
- Finite temperatures
- Full three dimensional treatment of magnetization in relativistic calculations including LDA+U.
- Non-collinear magnetism.
- Tight-binding regime.
- Hoppings integrals extraction regime.
- Optical Properties ( $\epsilon_1, \epsilon_2$ , reflectivity, electron energy loss spectra) using LMTO-ASA, LMTO full potential and tight-binding only regimes, with spin polarization, spin-orbit coupling, LDA+U included. (properly functioning when connected to MStudio MINDLab software.)
- Full 3D support for plotting charge densities, full potentials as well as full 3d magnetizations and magnetic fields (properly functioning when connected to MStudio MINDLab software.)
- Full 3D support for plotting Fermi surfaces and the Fermi velocities as vector fields (properly functioning when connected to MStudio MINDLab software.)
- Full 3D support for plotting crystal structures and orbitals (cubic/spherical harmonics) (properly functioning when connected to MStudio MINDLab software.)

[18]

The LmtART is written using FORTRAN 90. The input files to the LmtART involve in its simplest case only atomic charges of the atoms as well as crystal structure. LmtART can run in the fast regimes such as using atomic sphere approximation. LmtART can also run using tight-binding mode. To use this mode, only hopping integrals have to be specified. LmtART can also be used to withdraw tight-binding parameters from LDA calculation since tight-binding LMTO basis set is implemented inside the code. [18]

Further info: [http://www.physics.ucdavis.edu/~mindlab/MaterialResearch/Scientific/index\\_lmhart.htm](http://www.physics.ucdavis.edu/~mindlab/MaterialResearch/Scientific/index_lmhart.htm).

Development: The bulk of the program has been developed at the Max-Planck Institute for Solid State Research in Stuttgart, Germany. Extensions of LmtART were under development in Department of Physics, Rutgers University, Department of Physics, New Jersey Institute of Technology, and now in Department of Physics, University of Califor-

nia, Davis. [18]

### 3.1.11 OCTOPUS

Main characteristic: Ab initio.

Availability: Non commercial. Octopus is free software, released under the General Public License, so one is free to use it and modify it.

Introduction: Octopus is a scientific program aimed at the ab initio virtual experimentation on a hopefully ever increasing range of systems types. Electrons are described quantum-mechanically within the Density-Functional Theory (DFT), in its time-dependent form (TDDFT) when doing simulations in time. Nuclei are described classically as point particles. Electron-nucleus interaction is described within the Pseudopotential approximation. [19]

Theory

- Density Functional Theory for ground-state calculations: LDA, GGA and Optimized Effective Potential (OEP) functionals available through libxc.
- Time-dependent DFT for response

Systems

- Works in 1, 2, and 3 dimensions
- Periodic boundary conditions in 1, 2, or 3 directions (only for ground-state calculations)

Linear Response

- Through time-propagation: Static polarizabilities, Absorption spectra (singlet, triplet).
- Marc Casida's formulation of response: Electronic excitations
- Sternheimer (frequency dependent) linear-response formalism: Static and dynamic electric polarizabilities (including resonant response), Static and dynamic electric first hyperpolarizabilities (including resonant response), Static magnetic susceptibilities and Vibrational modes.

Non-linear response - Dynamics

- Ehrenfest dynamics for the nuclei
- Real-time TDDFT propagation.
- Emission spectra, harmonic generation
- Optimal control theory
- Car-Parrinello Molecular Dynamics

## Technical

- Norm-conserving pseudopotentials (most commonly used formats)
- Real-space grid discretization (no basis sets)
- Curvilinear coordinates
- Parallelization in domains and in states
- Runs both in single and double precision

[19]

### Further info:

[http://www.tddft.org/programs/octopus/wiki/index.php/Main\\_Page](http://www.tddft.org/programs/octopus/wiki/index.php/Main_Page)

Development: Current developers: Alberto Castro, Angel Rubio, Miguel A.L. Marques (hyllios), Micael Oliveira, Carlo Andrea Rozzi, Xavier Andrade, Danilo Nitsche, David Strubbe and Arto Sakko. Former developers: Florian Lorenzen and Heiko Appel. [19]

## **3.1.12 SIESTA**

Main characteristic: Ab initio.

Availability: Non commercial. License. SIESTA is distributed freely for individual academic users.

Introduction: SIESTA, Spanish Initiative for Electronic Simulations with Thousands of Atoms, is both a method and its computer program implementation, to perform electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. The fundamental idea behind the SIESTA formalism is to use localized orbitals of different symmetry to describe the wave functions of the electrons rather than using a planewave basis. It is a linear-scaling density-functional method. SIESTA is written in the programming language Fortran 90. [20] SIESTA is a ASE supported calculator. ASE is written in the programming language Python with the aim of setting up, steering and analyzing atomistic simulations. [7]

SIESTA routinely provides: total and partial energies; atomic forces; stress tensor; electric dipole moment; Atomic, orbital and bond populations (Mulliken); electron density. And also (though not all options are compatible): geometry relaxation, fixed or variable cell; constant-temperature molecular dynamics (nose thermostat); variable cell dynamics (Parrinello-Rahman); Spin polarized calculations (collinear or not); k-sampling of the Brillouin zone; local and orbital-projected density of states; band structure. [20]

Further info: <http://www.icmab.es/siesta/index.php>.

Development: Siesta Manager: Jose A. Torres. Main Siesta Developers: Emilio Artacho, José M. Cella, Julian Gale, Alberto García, Javier Junquera, Richard M. Martin, Pablo Ordejón, Daniel Sánchez-Portal, José M. Soler. [20]

### **3.1.13 STOBE**

Main characteristic: Ab initio.

Availability: Non commercial. Licensed, but cheap for academic users.

Introduction: The software package StoBe (Stockholm-Berlin) is a numerical program package to evaluate and analyze the electronic structure as well as spectroscopic and other properties of molecules and atom clusters. The approach is based on self-consistent solutions of the Kohn-Sham Density Functional Theory equations using a Linear Combinations of Gaussian-Type Orbitals (LCGTO) approach. The initial version of StoBe was based on the deMon program code, originally written under the direction of D. R. Salahub at the University of Montreal. StoBe has been re-developed in major parts where the present version offers as advanced features in particular

- the evaluation of near-edge-Xray-absorption-fine-structure and Xray emission spectra (NEXAFS, XES)

- use of molecular symmetry

- extended properties package

[21]

Further info: <http://w3.rz-berlin.mpg.de/~hermann/StoBe/index.html>.

Development: Authors: K. Hermann, Berlin (Germany) and L. G. M. Pettersson, Stockholm University (Sweden). [21]

### **3.1.14 VASP**

Main characteristic: Ab initio.

Availability: Non commercial. VASP is not public-domain or share-ware, and will be distributed only after a license contract has been signed. Inquiries must be send to Jürgen Hafner ( Juergen.Hafner@univie.ac.at). The inquiry should contain a short description of the short term research aims. [22]

Introduction: Vienna Ab-initio Simulation Package VASP is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane-wave basis set. The approach implemented in VAMP/VASP is based on a finite-temperature local-density approximation (with the free energy as variational quantity) and an exact evaluation of the instantaneous electronic ground state at each MD-step using efficient matrix diagonalization schemes and an efficient Pulay mixing. These techniques avoid all problems occurring in the original Car-Parrinello method which is based on the simultaneous integration of electronic and ionic equations of motion. The interaction between ions and electrons is described using ultrasoft Vanderbilt pseudopotentials (US-PP) or the projector augmented wave method (PAW). Both techniques allow a reduction of the necessary number of plane-waves per atom for transition metals and first row elements. Forces and stress can be easily calculated with VAMP/VASP and used to relax atoms into their groundstate. [22] VASP is a ASE supported calculator. ASE is written in the programming language Python with the aim of setting up, steering and analyzing atomistic simulations. [7]

Further info: <http://cms.mpi.univie.ac.at/vasp/>.

Development: In addition, the following people have contributed to the code: The tetrahedron integration method was copied from a Linear Muffin-Tin Orbitals (LMTO) program. The communication kernels were initially developed by Peter Lockey at Daresbury (CETEP), but they have been subsequently modified completely. The kernel for the parallel Fast Fourier Transform (FFT) was initially written by D. White and M. Payne, but it has been rewritten from scratch around July 1998. Several parts of VASP were co-developed by A. Eichler, and other members of the group in Vienna. David Hobbs worked on the non collinear version. Martijn Marsman has written the routines for calculating the polarization using the Berry phase approach, spin spirals and Wannier functions. He also rewrote the LDA+U routines initially written by O. Bengone, and extended the spin-orbit coupling to  $f$  electrons. Robin Hirschl implemented the Meta-GGA, and is currently working on the Hartree-Fock support (together with Martijn Marsman and Adrian Rohrbach). [22]

### **3.1.15 WIEN2K**

Main characteristic: Ab initio.

Availability: Non commercial. A small cover charge for academic institutions.

Introduction: The program package WIEN2k allows to perform electronic structure cal-



culations of solids using density functional theory. It is based on the full-potential (linearized) augmented plane-wave ((L)APW) and local orbitals (lo) method, which is one of the most accurate schemes for band structure calculations. WIEN2k is an all-electron scheme including relativistic effects and has many features. [23]

Further info: <http://www.wien2k.at/index.html>

### 3.1.16 ADF

Main characteristic: Ab initio.

Availability: Commercial, but cheaper for academic users.

Introduction: ADF, Amsterdam Density Functional software. ADF is based on Density Functional Theory (DFT). It consists of

- the molecular DFT program ADF
- the periodic DFT program BAND
- the post-ADF COSMO-RS program for thermodynamics of liquids

[24]

ADF and BAND can be applied to all elements in the periodic table, to molecules in the gas phase, in solvents, and on (metal) surfaces. ADF excels at hard problems in:

- spectroscopy
- structure and reactivity
- chemical analysis
- transition metals and heavy elements
- environment effects (solvents, proteins)

[24]

ADF runs in parallel and has a Graphical User Interface (GUI). [24]

Scientific benefits (functionality)

- Calculate spectroscopic properties (optical spectra, NMR, IR, ...)
- Accurate modern xc functionals (meta-GGA's, hybrids, dispersion-corrected)
- Relativistic methods: all-electron heavy-element calculations with self-consistent spin-orbit coupling
- Uses Slater functions for the whole periodic table
- Accurate periodic systems calculations with atomic orbitals

- Chemical analysis: bond energy decomposition, fragment orbitals, NBO, AIM, ELF, .. [24]

Further info: <http://www.scm.com/>.

Development: ADF has been developed over the past decades by the well-known groups in Amsterdam (Prof. Baerends group) and Calgary (Prof. Ziegler group). Since the mid-nineties SCM has developed into the coordinator of a wide network of academic ADF development groups. SCM is now an independent spin-off company of the Vrije Universiteit in Amsterdam. SCM maintains and (co-)develops the software and supports the ADF user community. [24]

### **3.1.17 CASTEP**

Main characteristic: Ab initio.

Availability: Commercial. Copies of Materials Studio and CASTEP can be purchased from Accelrys. If you are a UK academic then you qualify for the free academic version of CASTEP, which is available via UKCP from CCPForge.

Introduction: CASTEP is a software package which uses density functional theory to provide a good atomic-level description of all manner of materials and molecules. CASTEP gives information about total energies, forces and stresses on an atomic system, it calculates optimum geometries, band structures, optical spectra, phonon spectra and much more. Molecular dynamics simulations can also be performed. CASTEP code is portable and parallel. [25]

Further info: <http://www.castep.org/>

Development: CASTEP was originally created by Prof. M.C. Payne and subsequently developed by various UK academics, primarily from the TCM group in Cambridge. For various technical reasons, it was felt in 1999 that the original code was in need of a total re-design and re-write, and so the CASTEP Development Group was created to do just that, using modern coding styles and Fortran90. CASTEP is marketed commercially by Accelrys, along with Materials Studio, their graphical front end for MS Windows. In the United Kingdom there is an academic distribution, maintained by UKCP. [25]

### 3.1.18 CRYSTAL

Main characteristic: Ab initio.

Availability: Commercial, but cheaper for academic users.

Introduction: The CRYSTAL package performs ab initio calculations of the ground state energy, energy gradient, electronic wave function and properties of periodic systems. Hartree-Fock or Kohn-Sham Hamiltonians (that adopt an Exchange- Correlation potential following the postulates of Density-Functional theory) can be used. Systems periodic in 0 (molecules, 0D), 1 (polymers, 1D), 2 (slabs, 2D), and 3 dimensions (crystals, 3D) can be treated. In each case the fundamental approximation made is the expansion of the single particle wave functions ('Crystalline Orbital', CO) as a linear combination of Bloch functions (BF) defined in terms of local functions. The local functions are, in turn, linear combinations of Gaussian type functions (GTF) whose exponents and coefficients are defined by input. [26]

Further info: <http://www.crystal.unito.it/>

and a manual: <http://www.crystal.unito.it/Manuals/crystal06.pdf>.

### 3.1.19 DMOL3

Main characteristic: Ab initio.

Availability: Commercial.

Introduction: DMol<sup>3</sup> is a unique, accurate, and reliable density functional theory (DFT) quantum mechanical code for research in the chemicals and pharmaceutical industries. It combines computational speed with the accuracy of quantum mechanical methods to predict materials properties. DMol is extremely versatile and can be applied to research problems in the gas phase, solvent, and solid state, in chemistry, materials science, chemical engineering, and solid state physics. [27] DMol<sup>3</sup> features:

- Perform fast, accurate calculations on molecules and materials
- Predict structures, energies, reactivity, and more

[27]

Further info: <http://accelrys.com/products/materials-studio/modules/dmol3.html>.

### 3.1.20 FHI-AIMS

Main characteristic: Ab initio.

Availability: Commercial, but cheaper for academic users.

Introduction: FHI-aims is an all-electron electronic structure code and it bases on atom centered orbitals.

FHI-aims provides:

- Numeric atom-centered basis sets: Preconstructed for elements 1-102, from fast qualitative to meV-converged total energies.
  - Ready for massively parallel runs: seamless parallelization (time and memory) from desktop to (ten)thousands of CPUs.
  - Efficiency: all-electron accuracy at plane-wave/ pseudopotential-like cost, up to thousands of atoms.
  - Density functional theory (LDA, GGA, also spin-polarized) for molecules and solids: total energies; interatomic forces; structure optimization; Born-Oppenheimer molecular dynamics; vibrations and phonon dispersion (calculated from finite differences).
  - Exchange-correlation "beyond DFT" (currently, non-periodic geometries only): Hartree-Fock and hybrid functionals; Moller-Plesset perturbation theory (MP2) and Random Phase Approximation (RPA); GW approximation.
  - Output: electron densities, Kohn-Sham orbitals, band structures, densities of states, etc.
- [28]

Further info: <http://www.fhi-berlin.mpg.de/aims/>.

### 3.1.21 GAUSSIAN

Main characteristic: Ab initio.

Availability: Commercial, but cheaper for academic users.

Introduction: Gaussian 09 is the latest in the Gaussian series of programs. It provides state-of-the-art capabilities for electronic structure modelling. From the fundamental laws of quantum mechanics, Gaussian 09 predicts the energies, molecular structures, vibrational frequencies and molecular properties of molecules and reactions in a wide variety of chemical environments. [29]

Further info: [http://www.gaussian.com/g\\_prod/g09.htm](http://www.gaussian.com/g_prod/g09.htm)

### **3.1.22 ONETEP**

Main characteristic: Ab initio.

Availability: Commercial.

Introduction: ONETEP is a quantum mechanics-based program designed specifically for calculations on large systems, perhaps over 500 atoms. ONETEP brings the accuracy of density functional theory (DFT) to bear on systems such as protein-ligand complexes, grain boundaries, and nanoclusters-systems, which in the past, could only be treated by less accurate, approximate methods. [30]

ONETEP is a linear scaling DFT code, so the time required for a calculation increases linearly with the number of atoms, much more slowly than in conventional DFT approaches. Because of this feature, the program can be used to model very large systems. [30]

Applications of ONETEP include studies of surface chemistry, the configurations of large molecular systems, and the structure and energetics of nanotubes. ONETEP can also be used to study the properties of defects â vacancies, interstitials, substitution impurities, grain boundaries, and dislocations â in semiconductors and ceramic materials. [30]

Further info: <http://accelrys.com/products/materials-studio/modules/onetep.html>

### **3.1.23 PARAGAUSS**

Main characteristic: Ab initio.

Availability: Commercial.

Introduction: ParaGauss is a parallel DFT code for solving challenging electronic structure problems in chemistry, surface science, and the field of nanostructured materials. It is written in FORTRAN 90 language, parallelization is achieved through the use of a few communication primitives implemented on top of MPI. Among other features ParaGauss provides:

- Calculation of DFT energy and forces

- Geometry optimization and local search of transition state
  - Pseudopotentials as an atomic core substitute
  - Relativistic methods for heavy elements including treatment of spin-orbit interaction
- [31]

Further info: [http://www.theochem.tu-muenchen.de/welcome/index.php?option=com\\_content&task=view&id=61](http://www.theochem.tu-muenchen.de/welcome/index.php?option=com_content&task=view&id=61).

Development: Technical University of Munich by TCHARMm Component Collection for the SciTegic Platform . Belling, T. Grauschopf, S. Krüger, F. Nörtemann, M. Staufer, M. Mayer, V.A. Nasluzov, U. Birkenheuer, A. Hu, A. Matveev, A.V. Shor, M. Fuchs-Rohr, K. M. Neyman, D. I. Ganyushin, T. Kerdcharoen, A. Woiterski, S. Majumder, and N. Rösch.

[31]

## 3.2 TIGHT BINDING PROGRAMS

### 3.2.1 DFTB+

Main characteristic: Tight binding.

Availability: Non commercial. License. Free of charge?

Introduction: Density Functional based Tight Binding and more (DFTB+). The aim of the DFTB+ project is to create a highly modularised, but nevertheless fast and efficient stand alone Density Functional based Tight Binding (DFTB) implementation, containing all useful extensions, which had been implemented in several separate programs before now, and adding new useful features. The DFTB+ is written in the programming language Fortran 95. [32]

The most important features of the code are:

- Non self-consistent charge (Non-scc) and scc calculations (with expanded range of SCC accelerators): Cluster/ molecular systems, Periodic systems (arbitrary K-point sampling, band structure calc.).
- l-shell resolved calculations possible
- Spin polarised calculation (collinear spin)
- Geometry optimisation: Steepest descent, Conjugate gradient.
- Geometry optimisation constraints (in xyz-coordinates)
- Molecular dynamics (NVE and NVT ensembles)
- Improved finite temperature calculations

- Dispersion correction (van der Waals interaction)
  - Ability to treat f -electrons
  - LDA+U extension
  - QM/MM coupling with external point charges (smoothing possible)
  - OpenMP parallelisation
  - Automatic code validation (autotest system)
  - New user friendly, extensible input format (HSD or XML)
  - Dynamic memory allocation
  - Additional tool for generating cube files for charge distribution, molecular orbitals, etc. (Waveplot)
- [32]

Further info: <http://www.dftb-plus.info/home/> and a manual:

<http://www.dftb-plus.info/fileadmin/DFTB-Plus/public/dftb/current/manual.pdf>.

Development: The DFTB+ code is the successor of the old DFTB and Dylax codes, which were developed in Paderborn in the group of Professor Frauenheim. It is developed in the same group (but now in Bremen in the Bremen Center for Computational Materials Science). [33]

### 3.2.2 HOTBIT

Main characteristic: Tight binding.

Availability: Non commercial. Open source.

Introduction: HOTBIT is a density functional tight binding calculator for Python's ASE environment. The code is an implementation of charge-self-consistent density-functional tight-binding. HOTBIT code is written in the programming language Python. [34] ASE is written in the programming language Python with the aim of setting up, steering and analyzing atomistic simulations. [7]

Further info: <https://trac.cc.jyu.fi/projects/hotbit/>.

Development: HOTBIT code was written in NanoScience Center, University of Jyväskylä, Finland by Pekka Koskinen and friends. The predecessor of the code is Fortran-based tight-binding code, originally initiated by Michael Moseler, Fraunhofer IWM, Freiburg. [34]

### 3.2.3 PLATO

Main characteristic: Tight binding.

Availability: Non commercial. License. Free of charge? Contact Andrew Horsfield or Steven Kenny.

Introduction: Plato is the Package for Linear-combination of Atomic Orbitals. It allows one to perform molecular dynamics, structure optimisation etc using atomic orbital based electronic structure methods tight binding and density functional theory. [35]

Further info: <http://www.platoprogram.net/>.

### 3.2.4 TB-LMTO-ASA

Main characteristic: Tight binding.

Availability: Non commercial. Free of charge.

Introduction: The Stuttgart TB-LMTO-ASA program is in use world wide because it is extremely fast, user-friendly, hardware-independent, and free of charge. The program delivers tools for analysing the electronic structure and chemical bonding such as: Orbital-projected band structures, Crystal Orbital Hamiltonian Populations (COHP)s for describing bond strengths, and electron localization functions (ELFs). The division of space into potential-spheres is done automatically. Input is the crystal structure and output is the charge- and spin-selfconsistent band structure, the partial densities of states, the Fermi surface, plots of the full charge and spin-densities, the total energy, and the partial pressures. [36]

Further info: <http://www.fkf.mpg.de/andersen/>

Development: The development of the TB-LMTO-ASA program has been managed by Ole Krogh Andersen; the first version was constructed mostly by Mark van Schilfgaarde during 1987-88. Over the years the following people (in alphabetic order) have written, corrected or made additions to the program: Vladimir Antonov, Peter Braun, Armin Burkhardt, Volker Eyert, Georges Krier, Toni A. Paxton, Andrei Postnikov, Andreas Savin, R. W. Tank. The latest major revisions and additions are due to O. Jepsen and O. K. Andersen. [36]



## 3.3 CLASSICAL MOLECULAR DYNAMICS PROGRAMS

### 3.3.1 AMBER

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Licensed, but cheaper for academic users.

Introduction: "Amber" refers to two things: a set of molecular mechanical (MM) force fields for the simulation of biomolecules (which are in the public domain, and are used in a variety of simulation programs); and a package of molecular simulation programs which includes source code and demos. The current Amber code version is 10. A good general overview of the Amber codes can be found in: D.A. Case, T.E. Cheatham, III, T. Darden, H. Gohlke, R. Luo, K.M. Merz, Jr., A. Onufriev, C. Simmerling, B. Wang and R. Woods. The Amber biomolecular simulation programs. *J. Computat. Chem.* 26, 1668-1688 (2005). [37]

Further info: <http://ambermd.org/>.

Development: Amber is developed in an active collaboration of David Case at Rutgers University, Tom Cheatham at the University of Utah, Tom Darden at NIEHS, Ken Merz at Florida, Carlos Simmerling at SUNY-Stony Brook, Ray Luo at UC Irvine, and Junmei Wang at Encysive Pharmaceuticals. Amber was originally developed under the leadership of Peter Kollman, and Version 9 is dedicated to his memory. [37]

### 3.3.2 CHARMM

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Licensed, but cheaper for academic users.

Introduction: CHARMM (Chemistry at HARvard Macromolecular Mechanics) is a program for macromolecular simulations, including energy minimization, molecular dynamics and Monte Carlo simulations. [38] With the CHARMM Component Collection, you can create customized simulation work flows that include:

- Assign forcefield types and parameters
- Score docked ligands using the Molecular Mechanics-Poisson Boltzmann with the Surface Area (MM-PBSA) or Molecular Mechanics-Generalized Born with Surface Area (MM-GBSA) method

- Dock ligands using the CDOCKER method
  - Run customized scripts created with the CHARMM scripting language
  - Perform molecular mechanics and molecular dynamics on proteins or protein-ligand complexes using a variety of forcefields, methods and solvent models
- [39]

Further info: <http://accelrys.com/products/scitegic/component-collections/charmm.html> and <http://yuri.harvard.edu/>

Development: The CHARMM Development Project involves a network of developers in the United States and elsewhere working with Professor Karplus and his group at Harvard to develop and maintain the CHARMM program. [38]

### 3.3.3 DESMOND

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Desmond and its source code are available without cost for non-commercial use by universities and other not-for-profit research institutions. A license for the commercial use of Desmond is available from Schrödinger, LLC.

Introduction: Desmond is a software package for performing high-speed molecular dynamics simulations of biological systems on conventional commodity clusters. The code uses novel parallel algorithms and numerical techniques to achieve high performance and accuracy on platforms containing a large number of processors, but may also be executed on a single computer. Desmond can compute energies and forces for many standard fixed-charged force fields used in biomolecular simulations, the parameters for which can be assigned using a template-based parameter assignment tool. Desmond is also compatible with polarizable force fields based on the Drude formalism. A variety of integrators and support for various ensembles have been implemented in the code, including methods for thermostating (Andersen, Nose-Hoover, and Langevin) and barostating (Berendsen, Martyna-Tobias-Klein, and Langevin). Ensembles typically used in membrane simulations (constant surface area and surface tension) and semi-isotropic and fully anisotropic pressure coupling schemes are also available. [40]

Desmond supports algorithms typically used to perform fast and accurate molecular dynamics. Long-range electrostatic energy and forces are calculated using particle-mesh-based Ewald techniques. Constraints, which are enforced using a variant of the SHAKE

algorithm, allow the time step to be increased. These approaches can be used in combination with time-scale splitting (RESPA-based) integration schemes. [40]

The Desmond software includes tools for minimization and energy analysis (which can be run efficiently in a parallel environment); methods for restraining atomic positions as well as molecular configurations; support for a variety of periodic cell configurations; and facilities for accurate checkpointing and restart. [40]

Desmond can also be used to perform absolute and relative free energy calculations. Other simulation techniques (such as replica exchange) are supported through a plug-in-based infrastructure, which also allows users to develop their own simulation algorithms and models. [40]

Desmond is integrated with a molecular modeling environment for setting up simulations of biological and chemical systems, and is compatible with widely used tools for trajectory viewing and analysis. [40]

Further info: [http://www.deshawresearch.com/resources\\_desmond.html](http://www.deshawresearch.com/resources_desmond.html).

Development: D. E. Shaw Research.

### **3.3.4 DL POLY**

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. DL\_POLY is supplied to individuals under an academic licence, which is free of cost to academic scientists pursuing scientific research of a non-commercial nature.

Introduction: DL\_POLY is a general purpose serial and parallel molecular dynamics simulation package. Two versions of DL\_POLY are currently available. DL\_POLY\_2 is the original version which has been parallelised using the Replicated Data strategy and is useful for simulations of up to 30,000 atoms on 100 processors. DL\_POLY\_3 is a version which uses Domain Decomposition to achieve parallelism and is suitable for simulations of order 1 million atoms on 8-1024 processors. Both versions are supplied together under one DL\_POLY licence. [41]

Further info: [http://www.cse.scitech.ac.uk/ccg/software/DL\\_POLY/index.shtml](http://www.cse.scitech.ac.uk/ccg/software/DL_POLY/index.shtml).

Development: The package is developed at Daresbury Laboratory by W. Smith, T.R.

Forester and I.T. Todorov. The original package was developed by the Molecular Simulation Group (now part of the Computational Chemistry Group, MSG) at Daresbury Laboratory under the auspices of the Engineering and Physical Sciences Research Council (EPSRC) for the EPSRC's Collaborative Computational Project for the Computer Simulation of Condensed Phases (CCP5). Later developments were also supported by the Natural Environment Research Council through the eMinerals project. The package is the property of the Central Laboratory of the Research Councils. [41]

### 3.3.5 DL MULTI

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. DL\_MULTI is supplied to individuals under an academic licence, which is free of cost to academic scientists pursuing scientific research of a non-commercial nature.

Introduction: This package allows molecular dynamics simulation of rigid molecules with the electrostatics described by a distributed multipole. It is based on the DL\_POLY simulation package. The modifications were written by M. Leslie who was in the the Molecular Simulation Group (now part of the Computational Chemistry Group, MSG) at Daresbury Laboratory under the auspices of the Engineering and Physical Sciences Research Council (EPSRC) for the EPSRC's Collaborative Computational Project for the Computer Simulation of Condensed Phases (CCP5). [42]

Further info: [http://www.cse.scitech.ac.uk/ccg/software/DL\\_MULTI/](http://www.cse.scitech.ac.uk/ccg/software/DL_MULTI/).

### 3.3.6 FHI96MD

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Permission to use and copy this software and its documentation is granted without fee.

Introduction: Ab-initio total-energy calculations are a powerful tool to describe and analyze precisely equilibrium as well as non-equilibrium properties of a broad class of materials. The FHI96MD program is an efficient code to perform molecular dynamics simulations and total-energy calculations for molecules, perfect crystals, defects, surfaces,

interfaces and dislocations in crystals for materials as different as semiconductors, simple and transition metals, insulators, etc. The program employs density-functional theory, first-principles pseudopotentials, and a plane-wave basis set. It has been specifically designed for large systems by optimizing memory usage and speed. [43]

Further info: <http://www.fhi-berlin.mpg.de/th/fhi96md/code.html>.

### 3.3.7 GROMACS

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. GROMACS is Free Software, available under the GNU General Public License.

Introduction: GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles. It is primarily designed for biochemical molecules like proteins and lipids that have a lot of complicated bonded interactions, but since GROMACS is extremely fast at calculating the nonbonded interactions (that usually dominate simulations) many groups are also using it for research on non-biological systems, e.g. polymers. GROMACS supports all the usual algorithms you expect from a modern molecular dynamics implementation, but there are also quite a few features that make it stand out from the competition: GROMACS provides extremely high performance compared to all other programs. A lot of algorithmic optimizations have been introduced in the code; we have for instance extracted the calculation of the virial from the innermost loops over pairwise interactions, and we use our own software routines to calculate the inverse square root. GROMACS can be run in parallel, using standard MPI communication. [44]

Further info:

New webpage: <http://www.gromacs.org/>, old webpage: <http://oldwww.gromacs.org/> and old wikipedia: [http://oldwiki.gromacs.org/index.php/Main\\_Page](http://oldwiki.gromacs.org/index.php/Main_Page)

Development: GROMACS was first developed in Herman Berendsens group, department of Biophysical Chemistry of Groningen University. It is a team effort, with contributions from several current and former developers all over world. We would also be happy to consider your contributions if they are of reasonably high quality!

Head authors & project leaders: Erik Lindahl (Stockholm Center for Biomembrane Research, Stockholm, SE), David van der Spoel (Biomedical Centre, Uppsala, SE), Berk

Hess (Max Planck Institute for Polymer Research, Mainz, DE).

Other current developers: Gerrit Groenhof (Max Planck Institute for Biophysical Chemistry, Göttingen, DE), Carsten Kutzner (Max Planck Institute for Biophysical Chemistry, Göttingen, DE).

Former developers: Emile Apol, Henk Bekker, Herman Berendsen, Aldert van Buuren, Rudi van Drunen, Anton Feenstra, Bert de Groot, Pieter Meulenhoff, Alfons Sijbers, Peter Tieleman.

[44]

### 3.3.8 GROMOS

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Licensed, but cheaper for academic users.

Introduction: GROMOS: Dynamic Modelling of Molecular Systems. GROMOS is a general purpose molecular dynamics computer simulation package for the study of biomolecular systems. Its purpose is threefold:

- Simulation of arbitrary molecules in solution or crystalline state by the method of molecular dynamics (MD), stochastic dynamics (SD) or the path-integral method.
- Energy minimization of arbitrary molecules.
- Analysis of conformations obtained by experiment or by computer simulation.

[45]

The simulation package comes with the GROMOS force field (proteins, nucleotides, sugars, etc.) the quality of which should be judged from the scientific literature concerning its application to chemical and physical systems, ranging from glasses and liquid crystals to polymers and crystals and solutions of biomolecules. [45]

Interesting applications of GROMOS96 (the latest version of GROMOS) are:

- prediction of the dependence of a molecular conformation on the type of environment (water, methanol, chloroform, DMSO, apolar solvent, crystal, etc.)
- calculation of relative binding constants by evaluating free energy differences between various molecular complexes using thermodynamic integration, perturbation and extrapolation
- prediction of energetic and structural changes caused by modification of amino acids in enzymes or of base pairs in DNA

- derivation of three-dimensional (3D) molecular structure on the basis of NMR data by using restrained MD techniques including time-averaged distance- and J-value restraining
  - dynamic modelling of molecular complexes by searching configuration space using MD or SD in 3- or 4-dimensions, soft-core interaction, local elevation search
  - prediction of properties of materials under extreme conditions of temperature and pressure, which may be experimentally inaccessible
- [45]

Further info: <http://www.igc.ethz.ch/GROMOS/whatisgromos>.

### 3.3.9 HIPPO

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Free of charge.

Introduction: Hippo is a software package for simulation and analysis of bio-molecules at an atomic level. It has been specifically developed for very efficient protein folding studies in aqueous and membrane environments. The code is very fast due to optimized and hand-coded assembly routines which make use of fast multi-media instructions on modern x86 cpus. Hippo is (partially) parallelized (using industry-standard OpenMP).  
[46]

Simulation methods

- Molecular dynamics (MD) in NVT, NPT, NVE ensembles
- Metropolis Monte Carlo (MC) in NVT and NPT ensembles
- Replica exchange with MD and MC

[46]

Further info: <http://biowerkzeug.org/index.php/Hippo> and <http://www.biowerkzeug.com/>

### 3.3.10 IMD

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Free of charge license.

Introduction: The ITAP Molecular Dynamics Program. IMD is a software package for classical molecular dynamics simulations. Several types of interactions are supported, such as central pair potentials, Embedded-Atom Method (EAM) potentials for metals, Stillinger-Weber and Tersoff potentials for covalent systems, and Gay-Berne potentials for liquid crystals. A rich choice of simulation options is available: different integrators for the simulation of the various thermodynamic ensembles, options that allow to shear and deform the sample during the simulation, and many more. There is no restriction on the number of particle types. [47]

The main design goals were to create a flexible and modular software reaching high performance on contemporary computer architectures, while being as portable as reasonably possible. IMD runs efficiently on both single processor workstations and massively parallel supercomputers, but is not very well suited for vector processors. The parallelization uses the standard MPI library for message passing. As IMD is written in ANSI C, it should be easily portable to any Unix-like environment. [47]

IMD supports the following types of short range interactions between atoms or molecules:

- tabulated central pair potentials
- Embedded-Atom (EAM) potentials for metals
- Stillinger-Weber and Tersoff potentials for covalent systems
- Gay-Berne potentials for nematic liquid crystals
- Except for Gay-Berne potentials, the number of different atom types is not limited.

[47]

Further info: <http://www.itap.physik.uni-stuttgart.de/~imd/index.html>

Development: IMD was originally developed by Jörg Stadler in the framework of subproject C14 Molekulardynamik von Quasikristallen of the Sonderforschungsbereich 382 Verfahren und Algorithmen zur Simulation physikalischer Prozesse auf Hochleistungsrechnern.

Jörg Stadler left the ITAP in summer 1997. Further contributors have been Erik Bitzek, Marco Brunelli, Dietmar Bunz, Martin Hohl, Christof Horn, Jutta Kaiser, Ralf Mikulla, Matthias Müller, Christoph Rudhart, Gunther Schaaf, Christian Ulrich, and Dieter Wolfangel.

The development of IMD is continued by a team including Peter Brommer, Franz Gähler, Christopher Kohler, Frank Pister, Johannes Roth, and Steffen Sonntag. Funding is now provided through the Collaborative Research Centre 716 ("Dynamic simulation of sys-



tems with large numbers of particles"), projects B1, B2, B5, and D2. [47]

### 3.3.11 KALYPSO

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Free of charge.

Introduction: Kalypso is a highly-visual Windows software package for molecular dynamics (MD) simulations of atomic collisions in (primarily) metallic and bimetallic crystals. Kalypso comprises a simulation engine of the same name, and various supporting utility programs. The physics of a MD simulation is encapsulated in the interatomic potential, which determines material dependent behavior such as melting, bond strengths, phonon properties, nuclear stopping, etc. Kalypso uses many-body potentials of the embedded atom method (EAM) type which can describe the material and cohesive properties of face-centered cubic (fcc) metals, hexagonal closest packed (hcp) metals, body-centered cubic (bcc) metals, some impurities in these metals, and bimetallic systems (alloys, films, clusters, multilayers). [48]

EAM potentials are not particularly suitable for modelling the cohesive and material properties of semiconductors like Si or GaAs, or ionic materials such as MgO. However, the short-range repulsive potentials for any binary compound material can be correctly simulated by Kalypso, which allows Kalypso to be used for energetic ion scattering simulations that are determined by hard collisions of a homo nuclear projectile species on any two-element material (e.g. Ar → KBr, O<sub>2</sub> → KBr). [48]

Typically, energy is imparted to the system by one or more primary projectiles such as an inert gas atom or a metal atom or cluster, or by temperature ramping. The range of particle energies that can be treated by Kalypso is roughly 0.1 eV to 10 keV. The lower energy limit is imposed by quantum effects, while the upper limit is determined by the treatment used for modelling inelastic effects, and by the practical difficulty of containing fast projectiles in nanoscale targets. This energy range covers, for example, deposition of metals by evaporation, sputtering and ion scattering phenomena, and numerous less familiar phenomena such as gamma-ray induced Doppler broadening. [48]

Most Kalypso simulations will involve the calculation of the average effects of N projectile impacts at a statistical sample of different surface impact points. Kalypso can

simulate these projectile impacts on a virgin surface ('zero-fluence' simulation) or on a surface which accumulates the damage from prior projectile impacts ('multiple impact' simulation). [48]

Kalypso will be of interest to researchers who are in the business of doing experiments with ions (e.g. ion bombardment, sputtering, ion scattering) that require interpretation in terms of an atomistic model, and to researchers of nanoscale phenomena in metallic systems. Kalypso can also be used to carry out theoretical inquiries of a more general nature that have no connection to particular experiments, e.g. how do sputtering at glancing and normal projectile incidence differ? [48]

Kalypso permits the modelling of the time evolution of a system that is defined by certain initial conditions and an interaction model. The simulation of events following each incident projectile trajectory is described as a 'run'. For example, a sputtering simulation might consist of 1000 runs, each lasting for 2000 fs. The initial conditions at the start of each run will be quite similar, except for the starting position (impact parameter) of the projectile, which will sample different impact points within the surface unit cell. [48]

The program uses the Verlet integration algorithm with an adaptive timestep to integrate the classical equations of motion for a system of interacting particles. The output from the simulation is a set of particle coordinates and velocities at one or more specified sampling intervals which are stored in the 'dynamics' (or 'trajectory') file. [48]

The next update of Kalypso, version 3.1 will be available in January 2010. [48]

Further info: <http://sites.google.com/site/kalypsosimulation/Home>.

Development: Marcus Karolewski, Sydney, Australia.

### **3.3.12 LAMMPS**

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. LAMMPS is distributed as an open source code under the terms of the GPL.

Introduction: Classical molecular dynamics code LAMMPS, an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for soft materials (biomolecules, polymers) and solid-state materials (metals, semiconductors) and

coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend. [49]

Kinds of systems LAMMPS can simulate:

- atomic (e.g. box of Lennard-Jonesium)
- bead-spring polymers
- united-atom polymers or organic molecules
- all-atom polymers, organic molecules, proteins, DNA
- metals
- granular materials
- coarse-grained mesoscale models
- ellipsoidal particles
- point dipolar particles
- hybrid combinations of these

[49]

Further info: <http://lammps.sandia.gov/>.

Development: LAMMPS is distributed by Sandia National Laboratories, a US Department of Energy laboratory. The core group of LAMMPS developers is Steve Plimpton, Paul Crozier, and Aidan Thompson. [49]

### **3.3.13 LPMD**

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Open source.

Introduction: Las Palmeras Molecular Dynamics, LPMD is a Molecular Dynamics (MD) code written from scratch in C++, as user-friendly, modular and multiplatform as possible. Some of its features are: it works using plug ins, it reads simple and intuitive configuration files, and includes utility software to perform analysis, conversion, and visualization of MD simulations. The latest stable version is 0.6.0. [50]

Further info: <http://www.gnm.cl/lpmd/pmwiki.php?n=Main.HomePage>.

### 3.3.14 MDRANGE

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Free of charge.

Introduction: The program is a molecular dynamics (MD) simulation program tailored for effective calculation of ion ranges. The word effective used here must be understood in the context of high-energy molecular dynamics calculations; if such a simulation only needs a few hours of CPU time to yield useful results, it can be considered very effective. [51] A brief summary of the physical principles used and features incorporated in version 1.52b of the program:

What it does

- Calculates ion ranges in solids
- Calculates deposited energies
- Calculates the primary recoil spectrum
- Obtaining stopping powers possible indirectly (see P. Haussalo et. al., NIM B 1996)
- Ion and sample elements which can be used: any
- Energy range in which calculation can be done: roughly 1 eV/amu - 10 MeV/amu
- Energy range in which use is justified: roughly 100 eV/amu - 100 keV/amu
- MDRANGE3.0: option for Puska-Echenique-Nieminen-Ritchie(PENR) electronic stopping model. Needs charge density file from user.
- MDRANGE3.0: option for Brandt-Kitakawa(BK)-electronic stopping model. Needs charge density file from user.

Algorithms

- Newtonian microcanonical formalism
- Smith-Harrison (Computers in Physics Sep/Oct 1989, 68 (1989)) solution of equations of motion.
- Variable time step which ensures stability in strong collisions
- Simulation cell atom moving with slices
- Recoil interaction approximation (RIA) used, i.e. only recoil atom interactions taken into account
- Initial state calculation to give realistic thermal displacements
- MDRANGE3.0: Damage build-up process using user-defined atom coordinates for different damage states.
- MDRANGE3.0: Simple sputtering caused surface erosion simulation using Sigmunds

linear theory.

Supported sample structures

- Initial atom coordinates read in from an input file
- Crystalline
- Amorphous
- Polycrystalline
- Multilayered combinations of crystalline and amorphous structures
- Random selection of crystalline or amorphous structure in multilayered structures
- An element and compound library in mdsetup

[51].

Further info: [http://beam.acclab.helsinki.fi/~knordlun/mdh/mdh\\_program.html](http://beam.acclab.helsinki.fi/~knordlun/mdh/mdh_program.html)

Development: Authors of the program V1.0 - V1.83b: Kai Nordlund, Accelerator Laboratory, University of Helsinki, Finland. Author of the user interface & some minor modifications: Jussi Sillanpää, September 1, 1994. Author of the program development from V1.X -> V3.0: Jarkko Peltola. Last update: Jarkko Peltola and Kai Nordlund, August 2002. [51]

### **3.3.15 MDYNAMIX**

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. The code is freely distributed under terms of GNU public license.

Introduction: MDynaMix is a Molecular Dynamics Program. Current version: 5.1 from 2 June 2008. It is a general purpose molecular dynamics code for simulations of mixtures of either rigid or flexible molecules, interacting by a force field consisting of Lennard-Jones, electrostatic, covalent bonds, angles and torsion angles potentials as well as of some optional terms, in a periodic rectangular, hexagonal or truncated octahedron cell. Rigid bonds are constrained by the SHAKE algorithm. In case of flexible molecular models the double time step algorithm is used. Algorithms for NVE, NVT and NPT statistical ensembles are implemented, as well as Ewald sum for treatment of the electrostatic interactions. Treatment of quantum correction to the atomic motion can be done within the Path Integral Molecular Dynamics approach. The program can be run both in sequential and parallel execution. The parallel version employs "replicated data" strategy. It can

be run on any parallel architecture or workstation cluster with MPI parallel environment installed. Trajectory analysis suite is included, as well as a module to perform expanded ensemble simulations (not yet parallelized). The code is highly universal. It uses only standard Fortran-77 statements and no external libraries (except MPI for parallel execution). [52]

Further info: <http://www.fos.su.se/~sasha/mdynamix/>.

Development: The program is originally based on the MOLDYN program by Aatto Laaksonen. Since 1993 many additional changes were made by Alexander Lyubartsev. [52]

### 3.3.16 MOIL

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Public domain.

Introduction: MOIL is a public domain molecular modelling software. Moil supports the usual set of tools for molecular modeling by classical mechanics, including energy calculations, energy minimization, molecular dynamics, and more. Code is available to simulate curve crossing within the Landau Zener model. Moil allows for reasonably straightforward conversion of PDB files to computable datasets (coordinate and energy templates). Besides standard applications MOIL evolves around the research in Ron Elber's laboratory. Examples are the Locally Enhanced Sampling Approach and reaction path and long time dynamics algorithms that are based on action optimization. Also included the recently developed Milestoning approach for the calculation of kinetics and thermodynamics along a reaction coordinate. The integration of a coarse-grained model into moil is yet another new feature of MOIL11. [53]

Further info: <http://cbsu.tc.cornell.edu/software/moil/moil.html>.

Development: MOIL11 team: Thomas Blom, Peter Majek, Serdal Kirmizialtin, and Ron Elber.

### 3.3.17 MOLDY

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Moldy is copyrighted and distributed under the GNU pub-

lic license.

Introduction: Moldy is a general-purpose molecular dynamics simulation program. It is sufficiently flexible that it ought to be useful for a wide range of simulation calculations of atomic, ionic and molecular systems. [54]

The system is specified at run time with a description file so there is no need to recompile when changing systems. The program handles much more of the bookkeeping than is traditionally done, keeping track of consistency of parameters, restart files, output trajectories and so forth. Sizing of arrays limits are all handled automatically. The source code may be obtained from the CCP5 program library in the usual way, and also directly from Oxford, with information about the latest release. [54]

#### Capabilities

- The program can handle any mixture of atoms or polyatomic molecules (linear or otherwise) of any size within the rigid-molecule approximation. There are no limits on the number of atoms in a molecule, the number of molecular species or number of molecules.
- The system can be in the liquid or solid state, with MD cells of arbitrary dimensions and angles.
- The simulation may be conducted at either constant volume or constant stress using the Parrinello-Rahman algorithm, and constant energy/enthalpy or constant temperature using Nose-Hoover.
- Interactions are by pair-potentials (based at atomic sites in the case of molecules) with or without coulombic interactions.
- Most common forms of potential functions are supported (Lennard-Jones, Buckingham, Born-Meyer, MCY) and the program is designed to make it very easy to add others.
- Short-ranged forces are handled using the link-cell method and the long-ranged coulombic forces by the Ewald sum.

#### Unusual Features

- Moldy does not use the usual "minimum-image" convention, but instead includes interactions between a molecule and ALL of its periodic images that lie inside the cut-off radius. This is more strictly correct and just as easy to implement as minimum-image because of the link-cell algorithm.
- Moldy incorporates a method of generating initial configurations for liquid systems called a "skew start". This can reliably generate a configuration which is partially ordered but avoids molecular overlap.
- There is a capability for defining a "framework" which is a rigid super-molecule per-

meating all of space. This may be used to model rigid surfaces or zeolite-like cages, for example.

[54]

**Analysis and Outputs:** The program incorporates radial distribution function calculations and running accumulation of many of the usual thermodynamic averages. Any more sophisticated analysis can be performed by storing configurational data throughout the run for later analysis. There are flexible facilities for doing this. In addition to the main program there are utilities for manipulating dump datasets. [54]

Further info: <http://www.ccp5.ac.uk/moldy/moldy.html>

### 3.3.18 NAMD

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. NAMD is distributed free of charge with source code.

Introduction: NAMD, recipient of a 2002 Gordon Bell Award, is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on Charm++ parallel objects, NAMD scales to hundreds of processors on high-end parallel platforms and tens of processors on commodity clusters using gigabit ethernet. NAMD uses the popular molecular graphics program Visual Molecular Dynamics (VMD) for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR. [55]

Software Setup:

- Precompiled binaries provided for 12 popular platforms.
- Installed at major NSF supercomputer sites.
- Portable to virtually any platform with ethernet or MPI.
- C++ source code and CVS access for modification.

Molecule Building:

- VMD used to prepare molecular structure for simulation.
- Also reads X-PLOR, CHARMM, AMBER, and GROMACS input files.
- Psfgen tool generates structure and coordinate files for CHARMM force field.
- Efficient conjugate gradient minimization.
- Fixed atoms and harmonic restraints.



- Thermal equilibration via periodic rescaling, reinitialization, or Langevin dynamics.

**Basic Simulation:**

- Constant temperature via rescaling, coupling, or Langevin dynamics.
- Constant pressure via Berendsen or Langevin Nose-Hoover methods.
- Particle mesh Ewald full electrostatics for periodic systems.
- Symplectic multiple timestep integration.
- Rigid waters and bonds to hydrogen atoms.

**Advanced Simulation:**

- Chemical and conformational free energy calculations.
- Locally enhanced sampling via multiple images.
- Tcl based scripting and steering forces.
- Analysis implemented as Tcl scripts in VMD.
- Interactive visual steering interface to VMD.

**Scalable Performance:**

- Based on the Charm++/Converse parallel runtime system.
- Spatial data decomposition for limited communication pattern.
- Message driven execution for latency tolerance on commodity networks.
- Measurement-based load balancing for scaling to hundreds of processors.
- Largest simulation to date is over 300,000 atoms on 1000 processors.

[55]

Further info: <http://www.ks.uiuc.edu/Research/namd/>.

Development: NAMD was developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign. [55]

### 3.3.19 NWCHEM

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. NWChem is available free of charge.

Introduction: NWChem provides many methods to compute the properties of molecular and periodic systems using standard quantum mechanical descriptions of the electronic wavefunction or density. In addition, NWChem has the capability to perform classi-

cal molecular dynamics and free energy simulations. These approaches may be combined to perform mixed quantum-mechanics and molecular-mechanics simulations. The NWChem source code tree current release is version 5.1. The Python programming language has been embedded within NWChem and many of the high level capabilities of NWChem can be easily combined and controlled by the user to perform complex operations. [56]

NWChem is a computational chemistry package designed to run on high-performance parallel supercomputers. Code capabilities include the calculation of molecular electronic energies and analytic gradients using Hartree-Fock self-consistent field (SCF) theory, Gaussian density function theory (DFT), and second-order perturbation theory. For all methods, geometry optimization is available to determine energy minima and transition states. Classical molecular dynamics capabilities provide for the simulation of macromolecules and solutions, including the computation of free energies using a variety of force fields. [56]

Further info: <http://www.emsl.pnl.gov/docs/nwchem/nwchem.html>.

Development: NWChem Contributors: E. J. Bylaska, W. A. de Jong, N. Govind, K. Kowalski, T. P. Straatsma, M. Valiev, D. Wang, E. Apra, T. L. Windus, J. Hammond, P. Nichols, S. Hirata, M. T. Hackler, Y. Zhao, P.-D. Fan, R. J. Harrison, M. Dupuis, D. M. A. Smith, J. Nieplocha, V. Tipparaju, M. Krishnan, Q. Wu, T. Van Voorhis, A. A. Auer, M. Nooijen, E. Brown, G. Cisneros, G. I. Fann, H. Fruchtl, J. Garza, K. Hirao, R. Kendall, J. A. Nichols, K. Tsemekhman, K. Wolinski, J. Anchell, D. Bernholdt, P. Borowski, T. Clark, D. Clerc, H. Dachsel, M. Deegan, K. Dyllal, D. Elwood, E. Glendenning, M. Gutowski, A. Hess, J. Jaffe, B. Johnson, J. Ju, R. Kobayashi, R. Kutteh, Z. Lin, R. Littlefield, X. Long, B. Meng, T. Nakajima, S. Niu, L. Pollack, M. Rosing, G. Sandrone, M. Stave, H. Taylor, G. Thomas, J. van Lenthe, A. Wong, and Z. Zhang. [56]

### **3.3.20 TINKER**

Main characteristic: Classical Molecular Dynamics.

Availability: Non commercial. Current Major Version: TINKER 5.0, release date: June 2009. This distribution version of TINKER, with full source code, is made available free of charge to anyone who wants it.

Introduction: The TINKER molecular modelling software is a complete and general pack-

age for molecular mechanics and dynamics, with some special features for biopolymers. TINKER has the ability to use any of several common parameter sets, such as Amber (ff94, ff96, ff98 and ff99), CHARMM (19 and 27), Allinger MM (MM2-1991 and MM3-2000), OPLS (OPLS-UA, OPLS-AA and OPLS-AA/L), Merck Molecular Force Field (MMFF), Liam Dang's polarizable potentials, and our own AMOEBA polarizable atomic multipole force field. Parameter sets for other standard force fields such as GROMOS, UFF, ENCAD and MM4 are under consideration for future releases. [57]

The TINKER package includes a variety of novel algorithms such as a new distance geometry metrization method that has greater speed and better sampling than standard methods, Elber's reaction path methods, several of our Potential Smoothing and Search (PSS) methods for global optimization, an efficient potential surface scanning procedure, a flexible implementation of atomic multipole-based electrostatics with explicit dipole polarizability, a selection of continuum solvation treatments including several variants of the generalized Born (GB/SA) model, the generalized Kirkwood implicit solvation model for AMOEBA, an interface to APBS for Poisson-Boltzmann calculations, an efficient truncated Newton (TNCG) local optimizer, surface areas and volumes with derivatives, a simple free energy perturbation facility, normal mode analysis, minimization in Cartesian, torsional or rigid body space, velocity Verlet stochastic dynamics, use of pairwise neighbor lists of an improved spherical energy cutoff method, Particle Mesh Ewald summation for partial charges and regular Ewald for polarizable multipoles, a novel reaction field treatment of long range electrostatics, and more.... [57]

Further info: <http://dasher.wustl.edu/tinker/>.

Development: The TINKER package has developed over a period of many years, very slowly during the late-1980s, and more rapidly since the mid-1990s in Jay Ponder's research group at the Washington University School of Medicine in Saint Louis. Many people have played significant roles in the development of the package into its current form. [57]

### **3.3.21 YASARA**

Main characteristic: Classical Molecular Dynamics.

Availability: Commercial, but cheaper for academic users.

Introduction: YASARA is a molecular-graphics, -modeling and -simulation program for

Windows, Linux and Mac OS X developed since 1993, that finally makes it really easy to answer your questions. With an intuitive user interface, photorealistic graphics and support for affordable shutter glasses, autostereoscopic displays and input devices, YASARA creates a new level of interaction with the 'artificial reality', that allows you to focus on your goal and forget about the details of the program. YASARA is rooted in the academic world. You can obtain the initial stage 'YASARA View' for free, while higher stages (YASARA Model, YASARA Dynamics, YASARA Structure) require a license fee [58]

Further info: <http://www.yasara.com/index.html>.

## **3.4 CLASSICAL MONTE CARLO PROGRAMS**

### **3.4.1 MMC**

Main characteristic: Classical Monte Carlo.

Availability: Non commercial. The program is distributed freely to academic users.

Introduction: MMC is a Metropolis Monte Carlo program for the simulation of molecular assemblies in the canonical, grand-canonical and isothermal-isobaric ensembles employing several convergence acceleration techniques (for example force-biased displacement, extension-biased and local torsion changes, preferential selection of solvent to be moved, cavity-biased insertion, virial-biased volume change). [59]

The simulated system generally consists of one part called solute and a collection of identical rigid molecules called solvent. The solute can consist of any number of molecules that can move freely and have any or all of their torsional degrees of freedom sampled. Bond lengths and bond angles are kept fixed. [59]

Solvation free-energy (change) can be calculated using thermodynamic integration, the perturbation formula, the overlap ratio method, the (cavity) Widom insertion method or by potential of mean force calculation using the adaptive umbrella sampling method. Both continuous deformation and creation/annihilation paths can be used. [59]

The solute environment can be analyzed based on the Proximity Criterion and the resulting analysis can be visualized by color coding the solute atoms based on selected analysis result. The Proximity Analysis can be also performed on Charmm or Amber trajecto-

ries. The calculations can use Charmm, Amber, Gromos, Gromacs, OPLS, EPEN and Clementi's potentials. Many atomtypes are built in, additional ones can be defined by the user. [59]

Further info: <http://atlas.physbio.mssm.edu/~mezei/mmc/>.

Development: Mihaly Mezei, Mount Sinai School of Medicine, New York. [59]

## 3.5 MICROMAGNETISM PROGRAMS

### 3.5.1 MAGPAR

Main characteristic: Micromagnetism.

Availability: Non commercial. Magpar is distributed under the terms of the GNU General Public License.

Introduction: Magpar is a finite element micromagnetics package which combines several features:

- Applicability to a variety of static and dynamic micromagnetic problems including uniaxial anisotropy, exchange, magnetostatic interactions and external fields
- Flexibility of the finite element method concerning the geometry and accuracy by using unstructured graded meshes
- Portability to different hardware platforms, which range from simple PCs to massively parallel supercomputers
- Scalability due to its highly optimized design and efficient libraries
- Versatility by including static energy minimization and dynamic time integration methods

[60]

Further info: <http://www.magpar.net/>.

Development: Werner Scholz.

### 3.5.2 NMAG

Main characteristic: Micromagnetism.

Availability: Non commercial. NMAG is released under the GNU General Public License

(GNU GPL) as published by the Free Software Foundation; either version 2, or (at your option) any later version.

Introduction: Nmag is a micromagnetic simulation package based on the general purpose multi-physics library nsim. [61]

Features in brief:

- based on finite elements (suitable for non-cuboidal structures)
- problem description in Python, therefore high degree of flexibility
- inbuilt mesh post processing tools
- efficient data storage (binary compressed) and extraction into vtk files (of course the raw data can be extracted)
- arbitrary crystal anisotropy
- (pseudo) periodic boundary conditions ("macro geometry approach")
- Spin torque transfer (Zhang-Li model for uniform current density)
- extensive documentation in html and pdf, including Tutorial
- download as source, debian package, (VMWare) virtual machine and bootable CD/DVD ISO image

[61]

Further info: <http://nmag.soton.ac.uk/nmag/>.

Development: Nmag is developed by the group of Hans Fangohr and Thomas Fischbacher in the School of Engineering Sciences at the University of Southampton. [61]

### 3.5.3 OOMMF

Main characteristic: Micromagnetism.

Availability: Non commercial. Public domain.

Introduction: The goal of the OOMMF (Object Oriented Micromagnetic Framework) project in the Information Technology Laboratory (ITL) at the National Institute of Standards and Technology (NIST) is to develop a portable, extensible public domain micromagnetic program and associated tools. This code will form a completely functional micromagnetics package, but will also have a well documented, flexible programmer's interface so that people developing new code can swap their own code in and out as desired. [62]

The original OOMMF solver, mmsolve2D, is based on a micromagnetic code that Mike Donahue and Bob McMichael had previously developed. It utilizes a Landau-Lifshitz ODE solver to relax 3D spins on a 2D square mesh, using FFT's to compute the self-magnetostatic (demag) field. Anisotropy, applied field and initial magnetization can be varied pointwise, and arbitrary shaped elements can be modeled. A new, fully 3D solver, Oxsii, is under development. [62]

Further info: <http://math.nist.gov/oommf/>

Development: The main contributors to OOMMF are Mike Donahue, and Don Porter. Further development status is active. [62]

## **3.6 LATTICE-BOLTZMANN AND FINITE ELEMENT METHOD PROGRAMS**

### **3.6.1 DL\_MESO**

Main characteristic: Lattice-Boltzmann.

Availability: Non commercial. DL\_MESO is supplied to individuals under an academic licence, which is free of cost to academic scientists pursuing scientific research of a non-commercial nature.

Introduction: DL\_MESO is a mesoscale simulation package. It is written in C++ and supports both Lattice Boltzmann (LB) and Dissipative Particle Dynamics (DPD) methods. It is supplied with its own java based Graphical User Interface (GUI) and is capable of both serial and parallel execution. [64]

Further info: [http://www.cse.scitech.ac.uk/ccg/software/DL\\_MESO/](http://www.cse.scitech.ac.uk/ccg/software/DL_MESO/),  
more info in the manual:

[http://www.cse.scitech.ac.uk/ccg/software/DL\\_MESO/MANUAL/USRMAN.pdf](http://www.cse.scitech.ac.uk/ccg/software/DL_MESO/MANUAL/USRMAN.pdf)

Development: R. Qin for CCP5 under a grant provided by EPSRC. [64]

## 3.7 OTHER PROGRAMS

### 3.7.1 MSINDO

Main characteristic: Semiempirical molecular orbital program.

Availability: Non commercial. The source code can be obtained by request.

Introduction: MSINDO is a semiempirical molecular orbital program for the calculation of molecular and condensed matter properties of systems with first-, second-, third- and fourth-row elements. It is a modification of the original SINDO1 method. The current version of MSINDO includes parameters for the following elements: H, Li-F, Na-Cl, K-Br. Calculation of elements Rb-I is now possible, but the parameterization is not yet complete. The program is parameterized with emphasis on ground state properties, mainly heats of formation, structure data, ionization energies and dipole moments. Ground state properties are calculated on the SCF level, excited states on the CIS level. The source code can be obtained by request. The program provides data of the following properties as output: geometries, binding energies, ionization potentials (vertical and  $\Delta$ SCF), dipole moments, zero point energies, heats of formation, vertical excitation energies, oscillator strengths, atomic charges (Mulliken and Löwdin), bond orders, atomic and bond valences, diradical and zwitterion character, molecular electrostatic potentials (MESP), and (less accurate) force constants and vibrational frequencies. In addition the program is suitable for the calculation of thermal and photochemical reactions and solvent effects. [65]

Bulk and surface simulations can be performed with an embedding procedure or within the Cyclic Cluster Model (CCM). Contributions from the Madelung potential are taken into account by the Ewald summation technique. [65]

Born-Oppenheimer molecular dynamics runs are now enabled for RHF, UHF, and ROHF. To accelerate the reaction processes and to evaluate the free energy barriers, the metadynamics technique is available. [65]

The programming language is Fortran90. Memory is allocated dynamically for large arrays and statically for small arrays and variables. MSINDO 3.2.1 can be compiled with most available Fortran90 and F95 compilers. [65]

Further info: <http://www.thch.uni-bonn.de/tc/index.php?section=downloads&subsection=MSINDO&lang=english>.



### 3.7.2 (SAT)LEED

Main characteristic: Comparison of experimental and calculated Low Energy Electron Diffraction (LEED) I/V-spectra.

Availability: Non commercial. The programs can be downloaded for free and may be freely used, but not distributed.

Introduction: Several LEED packages are available, with different capabilities. However, the symmetrized automated tensor LEED program (SATLEED) is most recommended, versatile and up-to-date of the packages. [66]

The Symmetrized Automated Tensor Low Energy Electron Diffraction (SATLEED) package was designed to evaluate electron diffraction data to determine a crystal surface structure by comparison of experimental and calculated LEED I/V-spectra. This is version 1.0 of the SatLeed GUI software. This package consists of three main parts: the SatLeed package – a serial version of a symmetric Tensor Leed program; the Parallel SatLeed code – a parallel version of the original serial SatLeed package; the Graphical User Interface (GUI) to the serial SatLeed package. SATLEED enables one to quickly explore a variety of bulk crystal structures, inspect and analyze local geometries and symmetries of any (h k l) oriented crystal surfaces, increase the SATLEED performance through parallelization in order to minimize the calculation time, investigate more complex crystal structures now possible due to the increased speedup and generate informative graphics of resulting crystal structures for presentations and publications. SATLEED is written in the programming language FORTRAN 77. [5]

SATLEED, like the other packages, should normally be supplemented by the phase shift package: the phase shifts are needed as input to the LEED calculations. The Barbieri/Van Hove phase shift calculation package is also available in the LEED calculation home page. [5]

The different LEED packages are the following: symmetrized automated tensor LEED programs (SATLEED), symmetrized automated tensor LEED programs for very COMPLEX structures (SATCLEED), multi-termination symmetrized automated tensor LEED programs for multiple coexisting surface structures (MSATLEED), non-symmetrized automated tensor LEED programs for multiple angles of incidence and/or surface structures (ATLMLEED), non-symmetrized automated tensor LEED programs (ATLEED), The conventional LEED programs - the Van Hove/Tong package (LEEDCON). [66]

Further info:

[http://www.ap.cityu.edu.hk/personal-website/Van-Hove\\_files/leed/leedpack.html](http://www.ap.cityu.edu.hk/personal-website/Van-Hove_files/leed/leedpack.html) and a manual: <http://www.cs.utk.edu/~samatova/LEED/manual.html>.

Development: SATLEED GUI software version 1.0 package consists of three parts. The first is the SATLEED package - a serial version of a symmetric tensor leed program developed by M.A. Van Hove, A. Barbieri, Rous, Wander and R. Doell. Second part is the parallel SatLeed code and the third is the graphical user interface (GUI). [5]

## **3.8 FURTHER PROGRAMS**

There is amount of programs, that come up during the search for the database, but nevertheless could not been added to it. For most of these there is a webpage known, where it's possible to find more information. All of these programs listed here are non commercial. In the end of this section there is a list of programs for which no webpage have been found.

### **3.8.1 LIST OF NON COMMERCIAL PROGRAMS**

ADUN: <http://cbbi.imim.es:8080/Adun>.

ATOMPAW/PWPAW: <http://www.wfu.edu/~natalie/papers/pwpaw/man.html>.

CASINO: <http://www.tcm.phy.cam.ac.uk/~mdt26/casino2.html>.

COLUMBUS: <http://www.univie.ac.at/columbus/>.

CP2K: <http://cp2k.berlios.de/>.

DIRAC: [http://wiki.chem.vu.nl/dirac/index.php/Dirac\\_Program](http://wiki.chem.vu.nl/dirac/index.php/Dirac_Program).

ELK FP-LAPW: <http://elk.sourceforge.net/>.

FIREFLY(former PC GAMESS): <http://classic.chem.msu.su/gran/gamess/index.html>.

FLAIR: <http://www.uwm.edu/~weinert/flair.html>.

GAMESS-UK: <http://www.cfs.dl.ac.uk/index.shtml>.

GAMESS-US: <http://www.msg.chem.iastate.edu/gamess/>.

HILAPW: <http://home.hiroshima-u.ac.jp/fpc/manuals/HiLAPW/HiLAPW.html>.

MOLCAS: <http://www.teokem.lu.se/molcas/>.

HOOMD-BLUE: <http://codeblue.umich.edu/hoomd-blue/index.html>.

MOPAC: <http://openmopac.net/>.

MOSCITO: <http://ganter.chemie.uni-dortmund.de/MOSCITO/>.

MPQC: <http://www.mpqc.org/index.php>.

OPENMX: <http://www.openmx-square.org/index.html>.  
PARATEC: <http://www.nersc.gov/projects/paratec/>.  
PARSEC: <http://parsec.ices.utexas.edu/index.html>.  
PSI3: <http://www.psicode.org/>.  
PYQUANTE: <http://pyquante.sourceforge.net/>.  
RKMAG: <http://www.rkmag.com/index.html>.  
SEQQUEST: <http://dft.sandia.gov/Quest/>.  
SOCORRO: <http://dft.sandia.gov/socorro/mainpage.html>.  
TOWHEE: <http://towhee.sourceforge.net/>.  
TRAMONTO: <https://software.sandia.gov/DFTfluids/>.  
QUANTUM-ESPRESSO: <http://www.quantum-espresso.org/index.php>.

### **3.8.2 PROGRAMS WITHOUT KNOWN WEBPAGE**

AKMC

ASSIMPOT

BIGDFT

MolSimu: The program is currently suspended while the request for its renewal is being processed.

CONQUEST

DALTON

DDD(Discrete Dislocation Dynamics)

DFT++

DYMOKA

ELSTRU

FINGER

GDM2

GRASP

GTOFF

LAKIMOCA

MBPP

MUPHY

PARCAS MD

PMD

PRIRODA04

## REFERENCES

- [1] Cost Action P19, [web document], available at: <http://www.ipm.cz/costp19/>, referred 19.8.2009.
- [2] A. Gross, Theoretical surface science -a microscopic perspective. Springer-Verlag, Berlin (2003).
- [3] Richard J. Sadus, Molecular simulations of fluids -Theory, algorithms and object-orientation. Elsevier Science B.V. Amsterdam (1999).
- [4] Y.W. Kwon, S. Hosoglu, Computers and Structures 86 (2008) 663-670.
- [5] SatLeed GUI Manual, [web document], available at: <http://www.cs.utk.edu/~samatova/LEED/manual.html>, referred 7.7.2009.
- [6] Abinit homepage, [web document], available at: <http://www.abinit.org/>, referred 7.7.2009.
- [7] Atomic Simulation Environment homepage, [web document], available at: <https://wiki.fysik.dtu.dk/ase/>, referred 15.7.2009.
- [8] Short presentation of the ABINIT project, [web document], available at: <http://www.abinit.org/about/presentation.pdf>, referred 5.8.2009.
- [9] ACES II Release 2.5.0, User Manual, [web document], available at: <http://www.qtp.ufl.edu/Aces2/man-aces2.pdf>, referred 15.7.2009.
- [10] Goss, J. P. and Shaw, M. J. and Briddon, P. R. "Marker-method calculations for electrical levels using Gaussian-orbital basis sets", Berlin Heidelberg: Springer-Verlag, 2007.
- [11] Aimpro.Abinitio, [web document], available at: <http://aimpro.ncl.ac.uk/>, referred 13.7.2009.
- [12] CPMD consortium page, [web document], available at: <http://www.cpmc.org/>, referred 7.8.2009.
- [13] Dacapo project homepage, [web document], available at: <http://dcwww.camd.dtu.dk/campos/Dacapo/>, referred 7.7.2009.
- [14] DeMon (density of Montréal), [web document], available at: [http://demon-software.com/public\\_html/program.html](http://demon-software.com/public_html/program.html), referred 7.8.2009.

- [15] Levente Vitos, Computational quantum mechanics for materials engineers -The EMTO method and applications. Springer-Verlag London Limited (2007).
- [16] FLEUR: The Jülich FLAPW code family , [web document], available at: <http://www.flapw.de/pm/index.php>, referred 7.8.2009.
- [17] GPAW wiki-webpage, [web document], available at: <https://wiki.fysik.dtu.dk/gpaw/index.html>, referred 6.7.2009.
- [18] LmtART - a Full Potential LMTO Program, [web document], available at: [http://www.physics.ucdavis.edu/~mindlab/MaterialResearch/Scientific/index\\_lmtart.htm](http://www.physics.ucdavis.edu/~mindlab/MaterialResearch/Scientific/index_lmtart.htm), referred 11.8.2009.
- [19] Octopus wiki page, [web document], available at: [http://www.tddft.org/programs/octopus/wiki/index.php/Main\\_Page](http://www.tddft.org/programs/octopus/wiki/index.php/Main_Page), referred 10.8.2009.
- [20] SIESTA 2.0.2 User's Guide, [web document], available at: <http://www.icmab.es/siesta/manuales/manual-2.0.2/index.html>, referred 6.7.2009.
- [21] Stobe web distribution, [web document], available at: <http://w3.rz-berlin.mpg.de/~hermann/StoBe/index.html>, referred 11.8.2009.
- [22] VASP the Guide, [web document], available at: <http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html>, referred 6.7.2009.
- [23] Wien2k, [web document], available at: <http://www.wien2k.at/index.html>, referred 6.8.2009.
- [24] Scientific Computing & Modelling-ADF, [web document:], available at: <http://www.scm.com/>, referred 6.8.2009.
- [25] Castep homepage, [web document], available at: <http://www.castep.org/>, referred 7.8.2009.
- [26] CRYSTAL06 User's Manual, [web document], available at: <http://www.crystal.unito.it/Manuals/crystal06.pdf>, referred 13.8.2009.
- [27] Accelrys -Dmol3, [web document], available at: <http://accelrys.com/products/materials-studio/modules/dmol3.html>, referred 7.8.2009.
- [28] FHI-aims, [web document], available at: <http://www.fhi-berlin.mpg.de/aims/>, referred 7.8.2009.

- [29] Gaussian 09, [web document], available at: [http://www.gaussian.com/g\\_prod/g09.htm](http://www.gaussian.com/g_prod/g09.htm), referred 6.8.2009.
- [30] Accelrys-ONETEP, [web document], available at: <http://accelrys.com/products/materials-studio/modules/onetep.html>, referred 6.8.2009.
- [31] ParaGauss front page, [web document], available at: [http://www.theochem.tu-muenchen.de/welcome/index.php?option=com\\_content&task=view&id=61](http://www.theochem.tu-muenchen.de/welcome/index.php?option=com_content&task=view&id=61), referred 14.7.2009.
- [32] DFTB+ User manual, [web document], available at: <http://www.dftb-plus.info/fileadmin/DFTB-Plus/public/dftb/current/manual.pdf>, referred 17.7.2009.
- [33] DFTB+, [web document], available at: <http://www.dftb-plus.info/home/>, referred 17.7.2009.
- [34] Hotbit, [web document], available at: <https://trac.cc.jyu.fi/projects/hotbit>, referred 15.7.2009.
- [35] Plato program, [web document], available at: <http://www.platoprogram.net/>, referred 6.8.2009.
- [36] Abteilung Andersen, [web document], available at: <http://www.fkf.mpg.de/andersen/Methods.html>, referred 7.7.2009.
- [37] Amber Home Page, [web document], available at: <http://ambermd.org/>, referred 11.8.2009.
- [38] CHARMM, [web document], available at: <http://yuri.harvard.edu/>, referred 11.8.2009.
- [39] Accelrys -Charmm, [web document], available at: <http://accelrys.com/products/scitegic/component-collections/charmm.html>, referred 11.8.2009.
- [40] Desmond, [web document], available at: [http://www.deshawresearch.com/resources\\_desmond.html](http://www.deshawresearch.com/resources_desmond.html), referred 12.1.2010.
- [41] The DL\_POLY Molecular Simulation Package, [web document], available at: [http://www.cse.scitech.ac.uk/ccg/software/DL\\_POLY/index.shtml](http://www.cse.scitech.ac.uk/ccg/software/DL_POLY/index.shtml), referred 11.8.2009.
- [42] DL\_MULTI - A DL\_POLY package to simulate rigid molecules with multipoles, [web document], available at: [http://www.cse.scitech.ac.uk/ccg/software/DL\\_MULTI/](http://www.cse.scitech.ac.uk/ccg/software/DL_MULTI/), referred 11.8.2009.

- [43] The FHI96MD Package, [web document], available at: <http://www.fhi-berlin.mpg.de/th/fhi96md/code.html>, referred 13.8.2009.
- [44] GROMACS: Fast, Free and Flexible MD, [web document], available at: <http://oldwww.gromacs.org/>, referred 7.8.2009.
- [45] ETH -The IGC -GROMOS, [web document], available at: <http://www.igc.ethz.ch/GROMOS/whatisgromos>, referred 13.8.2009.
- [46] HIPPO wikipege, [web document], available at: <http://biowerkzeug.org/index.php/Hippo>, referred 12.1.2010.
- [47] IMD -The ITAP Molecular Dynamics Program, [web document], available at: <http://www.itap.physik.uni-stuttgart.de/~imd/index.html>, referred 10.8.2009.
- [48] Kalypso Simulation package, [web document], available at: <http://sites.google.com/site/kalypsosimulation/Home>, referred 12.1.2010.
- [49] LAMMPS Molecular Dynamics Simulator, [web document], available at: <http://lammps.sandia.gov/>, referred 10.8.2009.
- [50] Las Palmeras Molecular Dynamics, [web document], available at: <http://www.gnm.cl/lpmd/pmwiki.php>, referred 22.9.2009.
- [51] The MDRANGE program, [web document], available at: [http://beam.acclab.helsinki.fi/~knordlun/mdh/mdh\\_program.html](http://beam.acclab.helsinki.fi/~knordlun/mdh/mdh_program.html), referred 10.8.2009.
- [52] MDynaMix: a Molecular Dynamics Program, available at: <http://www.fos.su.se/~sasha/mdynamix/>, referred 12.8.2009.
- [53] MOIL - A Public Domain Molecular Modeling Software, [web document], available at: <http://cbsu.tc.cornell.edu/software/moil/moil.html>, referred 12.1.2010.
- [54] Moldy, [web document], available at: <http://www.ccp5.ac.uk/moldy/moldy.html>, referred 10.8.2009.
- [55] NAMD Scalable molecular dynamics, [web document], available at: <http://www.ks.uiuc.edu/Research/namd/>, referred 11.8.2009.
- [56] NWChem, available at: <http://www.emsl.pnl.gov/docs/nwchem/nwchem.html>, referred 13.8.2009.

- [57] TINKER homepage, [web document], available at: <http://dasher.wustl.edu/tinker/>, referred 13.8.2009.
- [58] YASARA -Yet another scientific artificial reality application, [web document], available at: <http://www.yasara.com/index.html>, referred 12.1.2010.
- [59] MMC, [web document], available at: <http://atlas.physbio.mssm.edu/~mezei/mmc/>, referred 13.8.2009.
- [60] Magpar Project, [web document], available at: <http://www.magpar.net/>, referred 5.8.2009.
- [61] Nmag Computational Micromagnetism, [web document], available at: <http://nmag.soton.ac.uk/nmag/>, referred 11.8.2009.
- [62] OOMMF homepage, [web document], available at: <http://math.nist.gov/oommf/>, referred 7.8.2009.
- [63] PC Micromagnetics Simulator Release Beta 2.0, [web document], available at: <http://math.nist.gov/oommf/contrib/simulmag/>, referred 6.8.2009.
- [64] The DL\_MESO Mesoscale Simulation Package, [web document], available at: [http://www.cse.scitech.ac.uk/ccg/software/DL\\_MESO/](http://www.cse.scitech.ac.uk/ccg/software/DL_MESO/), referred 11.8.2009.
- [65] MSINDO (Version 3.2.1), [web document], available at: <http://www.thch.uni-bonn.de/tc/index.php?section=downloads&subsection=MSINDO&lang=english>, referred 11.8.2009.
- [66] LEED Calculation Home Page, [web document], available at: [http://www.ap.cityu.edu.hk/personal-website/Van-Hove\\_files/leed/leedpack.html](http://www.ap.cityu.edu.hk/personal-website/Van-Hove_files/leed/leedpack.html), referred 7.7.2009.
- [67] Antti Puisto, The initial oxidation of transition metal surfaces, Doctoral Thesis.
- [68] The Chemical physics of solid surfaces, edited by D.P. Woodruff, Elsevier science B.V., Netherlands, 2001.
- [69] Exact Muffin-Tin Orbitals (EMTO) Method, [web document], available at: [https://www-pls.llnl.gov/?url=about\\_pls-condensed\\_matter\\_and\\_materials\\_division-eos\\_materials\\_theory-methods-emto](https://www-pls.llnl.gov/?url=about_pls-condensed_matter_and_materials_division-eos_materials_theory-methods-emto), referred 7.7.2009.
- [70] L. Vitos, I.A. Abrikosov and B. Johansson, "Anisotropic Lattice Distortions in Random Alloys from First-Principles Theory", Phys. Rev. Lett. 87, 156401 (2001).



- [71] Asap Atomic simulation enviroment, [web document], available at:  
<https://wiki.fysik.dtu.dk/asap/Asap>, referred 7.7.2009.
- [72] AIMPRO Community web pages, [web document], available at:  
<http://aimpro.ncl.ac.uk/restricted1/>, referred 21.7.2009.