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0521815916 - Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods
Jorge Kohanoff
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ELECTRONIC STRUCTURE CALCULATIONS FOR SOLIDS AND MOLECULES: THEORY AND COMPUTATIONAL METHODS

Electronic structure problems are studied in condensed matter physics and theoretical chemistry to provide important insights into the properties of matter. This graduate level textbook describes the main theoretical approaches and computational techniques for studying the behavior of electrons in molecules and solids, from the simplest approximations to the most sophisticated methods.

The first part describes in detail the various theoretical approaches to calculating the electronic structure of solids and molecules, including density functional theory (DFT) and chemical methods based on Hartree–Fock theory. The basic approximations, adiabatic, classical nuclei, local density, and gradient corrections, are thoroughly discussed, and an in-depth overview of recent advances and alternative approaches in DFT is given.

The second part discusses the different practical methods proposed in order to solve the electronic structure problem computationally. This is developed in parallel for DFT and Hartree–Fock approaches, including a detailed discussion of basis sets and practical aspects of the main methods in use, including plane waves, Gaussian basis sets, and augmentation methods. The final chapters address the issues of diagonalization, self-consistency, and first-principles molecular dynamics simulations.

At variance with most books in this area, this textbook addresses graduate students in both physics and chemistry, and is intended to improve communication between the two communities. It also serves as a reference for researchers coming into the field.

JORGE KOHANOFF is Reader in Applied Mathematics and Theoretical Physics at Queen's University Belfast. Following study at the University of Buenos Aires and SISSA in Trieste, he worked with IBM in Zurich, Switzerland, and gained his Ph.D. from ETH-Zurich. He then spent some time as a post-doctoral research assistant in France, before leading the Electronic Structure and Computational Physics Programme at the International Centre for Theoretical Physics, Trieste, Italy. He has published over 50 papers, including contributions in computational methods and applications in electronic structure, statistical mechanics, and Car–Parrinello molecular dynamics simulations.

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A Clarisa, Anna, Elena, Tuta y Blanca

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Preface

Very often when a postgraduate student begins a research activity in a new field, she or he is presented with a partial view of the big picture, according to the arena where the research group carries out its activity. For the student this implies narrowing the focus to a class of systems such as molecules, surfaces, liquids, defects, or magnetic systems, and to concentrate on a particular theoretical approach and one or a few specific computational techniques out of the many possibilities available. All this is perfectly understandable and reasonable because it is very difficult to absorb rapidly the knowledge accumulated during many decades, since the pioneering work of Hartree, Fock, Slater, Thomas, Fermi, Bloch, Dirac, and Wigner in the twenties and thirties, until the most recent developments in areas such as electronic correlation. This knowledge is built up during many years of practice in the field, participating in schools, conferences, and workshops that promote exchange and collaboration between the different subareas, discussing advantages and disadvantages of different approaches with colleagues around the world, and keeping up with the latest developments in the literature.

Although many excellent books and reviews are available in areas such as density functional theory, solid state physics, quantum chemistry, electronic structure methods, and Car–Parrinello simulations, it is desirable to have all this reference material condensed in a single book that may be used by a fresh graduate student, by a postdoc who is moving into the field, or by a researcher with experience in one or a few subareas who wants to broaden her or his horizons. In this way the researcher can become familiar with the basic ideas and the most common theoretical approaches and approximations and, at the same time, learn about the various computational methods devised to solve the electronic structure problem in practice. A recent book by Richard Martin (*Electronic Structure: Basic Theory and Practical Methods*, Cambridge University Press, 2004) fills that gap especially in the area of solid state physics. The present book covers many of those

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issues, too. However, it is specifically oriented to both physicists and chemists, by describing methods used by the two communities to study solids, liquids, and molecules, and trying to make connections whenever possible.

This book is the result of the experience accumulated in practice and through organization and participation in electronic structure activities. Four institutions were fundamental in this respect: the Scuola Internazionale Superiore di Study Avanzati (SISSA) in Trieste, where I first met some of the main practitioners in the field like Michele Parrinello and Roberto Car, the International Centre for Theoretical Physics (ICTP) in Trieste, where I spent five years (1994–1999) organizing electronic structure and computational physics activities, the Centre Européen de Calcul Atomique et Moléculaire (CECAM) in Lyon, where I attended several workshops, and Queen's University Belfast (Northern Ireland), which gave me the possibility of devoting part of my time to the writing of this book. The germ of this book can be traced back to an invitation from Abhijit Mookerjee to lecture in a School he organized at the S. N. Bose Centre in Calcutta (India) in 1998. In previous years I had the chance to organize several activities at ICTP, where many lecturers kindly provided notes for the participants. I then thought it would be a good idea to try and put together this kind of material in a systematic and consistent fashion, and set off to prepare a set of notes for the Calcutta Workshop. Along the years I kept on revising and enriching these lecture notes, which were used as reference material for postgraduate courses. They were also on-line for the advantage of scientists around the world. It was my feeling, and it was also suggested by Mookerjee and other colleagues who read the notes, like Mariana Weissman and Pablo Ordejón, that it could be a good idea to use them as a starting point for a book. The chance eventually materialized when Mike Finnis mentioned these notes to Eoin O'Sullivan from Cambridge University Press, and he suggested that I put forward a proposal for this book.

I started in the field of electronic structure calculations in 1990 guided by Michele Parrinello and Giulia Galli at IBM Zurich. Through conversations with other members of the group I rapidly learnt about the diversity of the field, and realized that different groups tend to choose a specific theoretical approach according to their goals, expertise, and background. Usually, physicists prefer DFT and chemists favor Hartree–Fock-derived methods, although in recent times there have been numerous crossings from one to the other side, and the very existence of hybrid HF-DFT methods, and the combination of configuration interaction approaches with DFT, proves that the interaction between these two communities is very beneficial. By including both types of approach in this book, my intention was to make it useful to both communities. Although clearly biased towards DFT methods, it gives physicists a general idea of what type of calculations are carried out by chemists, and vice versa. At least as important is making

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theoretical approaches into practical schemes for calculating electronic properties of materials from first principles. This means devising an appropriate framework for implementing the Hartree–Fock or DFT methodologies in a computer. Here is where the various groups depart from each other. The field becomes more technical, and precise mathematical and numerical techniques acquire a prominent role. The second part of this book is an attempt to give a broad picture of the different methods available, but it also goes in detail into some areas such as the pseudopotential plane wave method and the Car–Parrinello approach.

The first part of this book, Chapters 1 to 5, contains theoretical material that covers from the very basic approximations up to the latest developments in the field of electronic correlation. Chapter 1 begins with an introduction to the problem of the structure of matter, discusses the adiabatic and classical nuclei approximations – which are often confused – and ends with the statement of the electronic structure problem. Chapter 2 is a conceptual introduction to the general problem of calculating the electronic structure of a many-electron system. The physical origin of correlation is qualitatively discussed and introduced at a simple level in the case of classical systems, and is then extended to electronic systems. *Ab initio* approaches used in the theoretical chemistry community are described in Chapter 3, starting from the Hartree–Fock approximation, and moving onto various ways of including correlation such as configuration interaction and Møller–Plesset perturbation theory. Density functional theory is introduced and discussed in detail in Chapter 4, while Chapter 5 is devoted to exchange and correlation within DFT. It begins with the local density and generalized gradient approximations (LDA and GGA), and covers up to the most recent meta-GGA and hybrid HF-DFT approaches. Next, this chapter focuses on topics somehow out of the main stream, presenting the state-of-the-art in DFT. This chapter intends to be a reference that condenses the present understanding of the most popular (and unpopular) approximations.

The second part of this book is devoted to practical methods. Chapter 6 begins by setting the general framework and discussing the main technical issues that arise in an actual calculation: the choice of a basis set for representing the electronic orbitals, and the choice between all-electron and pseudopotential methods. It then reviews some basic concepts from solid state physics, like the unit cell, Bloch's theorem, Brillouin zone, and how aperiodic systems can be treated in periodic cell calculations. Due to the enormous role played in the past two decades, Chapter 7 is devoted to the development of pseudopotential theory in great detail, and discusses the many issues that arise, such as the choice of atomic configuration, ghost states, and non-linear core corrections. At the end of this chapter there is a set of practical hints on how to construct pseudopotentials. Chapter 8 is concerned with basis sets. After setting the general framework for molecular and

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crystalline systems, it describes in detail plane wave and atom-centered basis sets, specializing in the case of Gaussians. Other approaches are also mentioned, and a final section is devoted to augmentation schemes such as the APW and MTO basis sets, together with their linearized versions. Chapter 9 reviews in more or less detail the different electronic structure methods generally used, from the KKR approach to all-electron methods based on augmentation spheres, and the pseudopotential plane wave approach. Then it focuses on methods based on atom-centered basis sets, specifically discussing some technical aspects related to the use of Gaussian basis sets. Chapter 10 uses the framework set in the previous chapters to discuss simplified approaches to the electronic problem such as tight-binding schemes normally used in solid state physics, and semiempirical schemes commonly used in the theoretical chemistry community like extended Hückel, CNDO, and MNDO. A connection between these two parallel worlds is attempted. Simpler approaches like bond order potentials and empirical force fields are also reviewed, hybrid QM-MM methods are described, and a final section is devoted to simplified, orbital-free density functionals. Chapter 11 is concerned with the issues of diagonalization and self-consistency, and the final chapter is devoted to the Car–Parrinello extended Lagrangian method for first-principles molecular dynamics simulations.

I would have liked to include some other topics in this book, such as quantum Monte Carlo methods, density functional perturbation theory, electronic excitations, and quantum nuclear effects, for the sake of completeness. Unfortunately they remained outside the book, but readers will surely have no difficulty in locating the appropriate literature.

Most of what is in this book I learnt from reading and listening to the main actors along the years. It would take several pages to name them all, with the almost certainty of forgetting to mention someone. I want to thank, however, a few people who helped me with parts of the manuscript. First is my long-time friend Andrés Saul, who patiently read the first four chapters of the manuscript and helped me with the tight-binding section. Next is Sasha Lozovoi, who checked Chapters 6 and 7 and provided me with useful data. Then is my good friend Nikitas Gidopoulos. We wrote together a chapter on DFT in a recent handbook, which constituted the basis for Chapters 4 and 5. Mike Finnis critically read the section on tight-binding methods, and Tony Paxton had to suffer me bothering him so many times trying to understand how muffin-tin orbitals are constructed. Thanks also to Bob Jones and David Vanderbilt for kindly providing figures for reproduction. Last, but not least, I want to thank my three mentors: Erio Tosatti, Michele Parrinello, and Ruth Lynden-Bell. I am largely indebted to the three of them for their generous guidance and friendship.

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I would also like to mention some people who involuntarily participated in this book by sharing their experience on various subjects with me. In no particular order, these are the people I first met in SISSA like Mario Tosi, Stefano de Gironcoli, Stefano Baroni, Raffaele Resta, Roberto Car, Annabella Selloni, Giorgio Pastore, Furio Ercolessi, and Guido Chiarotti. Then there are Giulia Galli, Pedro Serena, Franco Buda, Wanda Andreoni, Peter Blöchl, François Gygi, Jürg Hutter, Andrew Fisher, Michiel Sprik, Ursula Röthlisberger, Dominik Marx, Mark Tuckerman, Ali Alavi, Mike Klein, and Kari Laasonen, whom I met during my years at IBM Zurich. Jean-Pierre Hansen, Hong Xu, Enrico Smargiassi, and Carlo Pierleoni were some of my colleagues in Lyon, and the following people I met through the years, in different places and times: David Ceperley, Charusita Chakravarty, Pietro Ballone, Daniel Laría, Rob Coalson, Michael Methfessel, David Vanderbilt, Sandro Scandolo, Darío Estrín, Ruben Weht, Ricardo Migoni, Sergio Koval, Ezequiel Leiva, Barbara Montanari, Mariana Weissman, Stuart Murdock, Carlo Cavazzoni, Saverio Moroni, Pablo Ordejón, Jose Soler, Emilio Artacho, Daniel Sánchez-Portal, Hardy Gross, Tchavdar Todorov, Ron Cohen, Detlef Hohl, Mike Gillan, Graeme Ackland, Cristián Sánchez, Raul Cachau, Mario Del Popolo, Tristan Youngs, Peijun Hu, Paolo Giannozzi, Andy Görling, Stewart Clark, Paul Madden, Richard Martin, Alfredo Caro, Jorge Sofo, Gleb Gribakin, Jose Luis Martins, Renata Wentzcovitch, Abdallah Qteish, and my students Simone Selenu, Carlos Pinilla, and Iván Scivetti, who had to suffer (or enjoy?) my disappearance during the final stages of the writing of this book. Special thanks go to my first Ph.D. student, Giuseppe Colizzi, who forced me to study pseudopotential theory properly, and provided me with the figures that are shown in the corresponding chapter. Finally, I can never be grateful enough to Clarisa and my daughters Anna and Elena for their patience and encouragement. Now it is time to make up for all those boring weekends watching me working on this book!

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Symbols

Operators

$\hat{\mathcal{H}}$	Hamiltonian operator
$\hat{h}_e$	electronic Hamiltonian
$\hat{T}$	electronic kinetic energy operator
$\hat{T}_n$	nuclear kinetic energy operator
$\hat{U}_{\rm ee}$	electron–electron interaction
$\hat{V}_{\rm ne}$	electron–nuclear interaction
$\hat{V}_{\rm nn}$	nuclear–nuclear interaction
$\hat{V}_{\rm ext}$	external interaction acting on electrons
$\hat{h}_1(i)$	core Hamiltonian for electron i
$\hat{v}_2(i,j)$	electron–electron interaction between electrons i and j
$\hat{\mathcal{F}}$	Fock operator
$\hat{\mathcal{J}}_i$	Coulomb operator
$\hat{\mathcal{K}}_i$	exchange operator
$\hat{H}_{\rm KS}$	Kohn–Sham one-electron Hamiltonian operator
$\hat{V}_{\rm PS}$	pseudopotential electron–nuclear interaction
$\hat{I}$	identity operator
$\hat{P}_l$	projection operator onto angular momentum l subspace
$\hat{S}$	overlap operator

Energy contributions

T	electronic kinetic energy
$U_{\rm ee}$	electron–electron interaction energy
$E_{\rm X}$	exchange energy
$E_{\rm C}$	correlation energy
$E_{\rm XC}$	exchange and correlation energy
$\tilde{E}_{\rm XC}$	coupling constant averaged exchange and correlation energy
$E_{\rm H}$	Hartree (direct Coulomb) energy
$V_{\rm ne}$	electron–nuclear interaction energy
$V_{\rm nn}$	nuclear–nuclear interaction energy

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V_{ext}	interaction energy of electrons with external sources
E_{KS}	Kohn–Sham energy
T_{R}	non-interacting electronic kinetic energy
K_{e}	fictitious kinetic energy in CPMD

Integrals in Hartree–Fock theory

E_{ii}	one-electron integrals
J_{ij}	Coulomb integrals
K_{ij}	exchange integrals

Potentials

$v_{\text{ext}}(\mathbf{r})$	external potential acting on electrons
$v_{\text{H}}(\mathbf{r})$	Hartree electrostatic potential
$\mu_{\text{XC}}(\mathbf{r})$	exchange-correlation potential
$v_{\text{KS}}(\mathbf{r})$	Kohn–Sham potential
$v_{\text{PS}}(\mathbf{r})$	pseudopotential

System specifications and constants

P	number of particles (atoms or nuclei)
M_I	mass of particle I
Z_I	charge of particle I
$\mathbf{R}_I$	coordinates of particle I
$\mathbf{R}$	coordinates of all the nuclei
N	number of electrons
m	mass of the electron
e	charge of the electron
$\mathbf{r}_i$	coordinates of electron i
$\mathbf{r}$	coordinates of all the electrons
$\mathbf{x}_i$	combined spatial and spin coordinates of electron i
$\hbar$	Planck's constant
ϵ_{F}	Fermi energy

Wave functions and eigenvalues

$\Psi_n(\mathbf{R},\mathbf{r}),\ \lvert\Psi_n\rangle$	total (electron–nuclear) wave function
$\mathcal{E}_n$	total (electron–nuclear) energy
$\Theta_n(\mathbf{R}),\ \lvert\Theta_n\rangle$	nuclear wave function
$\Phi_n(\mathbf{R},\mathbf{r}),\ \lvert\Phi_n\rangle$	electronic wave function
$E_n(\mathbf{R})$	electronic eigenstates
$\varphi_i(\mathbf{r}),\ \lvert\varphi\rangle$	one-electron orbitals
ε_i	one-electron eigenvalues
f_i	occupation numbers
$\psi_{\mathbf{k}}(\mathbf{r}),\ \lvert\psi_{\mathbf{k}}\rangle$	one-electron wave function of momentum $\mathbf{k}$
$\varepsilon(\mathbf{k})$	electronic dispersion relation
$\phi_\alpha(\mathbf{r}),\ \lvert\phi_\alpha\rangle$	generic basis function
M	size of the basis set

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Notation for crystalline systems

$\mathbf{a}_i$	lattice vectors
$\mathbf{T}$	lattice translations
$\mathbf{b}_i$	reciprocal lattice vectors
$\mathbf{G}$	reciprocal lattice translations
$\mathbf{k}$	wave vector in the first Brillouin zone
Γ-point	Brillouin zone center
$N_{\mathbf{k}}$	number of wave vectors in the first Brillouin zone
$\omega_{\mathbf{k}}$	weight of wave vector $\mathbf{k}$ in BZ sums
Ω	volume of unit cell or supercell
E_{cut}	plane wave energy cutoff
$S(\mathbf{G})$	structure factor

Density functionals

$f[\rho]$	functional
$\delta f[\rho]/\delta\rho(x)$	functional derivative
$\epsilon_{\text{XC}}[\rho]$	exchange-correlation energy density
$F_{\text{XC}}[\rho]$	exchange-correlation enhancement factor
$\tau[\rho]$	kinetic energy density

Density and response functions

$\rho(\mathbf{r})$	electronic density
$\zeta(\mathbf{r})$	spin-polarization or magnetization density
$\rho_1(\mathbf{r},\mathbf{r}')$	one-body density matrix
$\rho_2(\mathbf{r},\mathbf{r}')$	two-body density matrix
$g(\mathbf{r},\mathbf{r}')$	pair correlation function
$\tilde{g}(\mathbf{r},\mathbf{r}')$	coupling-constant-averaged pair correlation function
$\rho_{\text{XC}}(\mathbf{r},\mathbf{r}')$	exchange-correlation hole
$\chi_\sigma(\mathbf{r},\mathbf{r}')$	linear response function for spin σ
$G_\sigma(\mathbf{r},\mathbf{r}';E)$	Green's function for spin σ and energy E
$\Sigma(\mathbf{r},\mathbf{r}';E)$	self-energy
$W(\mathbf{r},\mathbf{r}';E)$	screened interaction

Atomic quantities

n, l, m	principal, angular, and magnetic quantum numbers
$\Phi_{\text{AE}}^{nlm}(r)$	all-electron atomic wave function
$Y_{lm}(\theta,\phi),\ \|lm\rangle$	spherical harmonic function
$P_l(\cos\theta)$	Legendre polynomial
$R_{nl}(r),\ \chi^l(r)$	radial component of the atomic wave function
$u^l(r)$	$r\chi^l(r)$
$\Phi_{\text{PS}}^{lm}(r)$	pseudo-atomic wave function
$\|\zeta^{lm}\rangle,\ \|\xi^{lm}\rangle,\ \|\beta^{lm}\rangle$	pseudopotential projector functions
$\eta_l(\varepsilon)$	phase shift
ζ_{nl}	exponents of Slater-type and Gaussian-type orbitals
$G_{ijk}(\mathbf{r},\alpha,\mathbf{R}_I)$	primitive Cartesian Gaussian

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Notation for atom-centered and augmented basis sets

$\mathbf{H}$, $H_{\alpha\beta}$	Hamiltonian matrix
$\mathbf{F}$, $F_{\alpha\beta}$	Fock matrix
$\mathbf{S}$, $S_{\alpha\beta}$	overlap matrix
$T^{IJ}_{\mu\nu}$	kinetic energy matrix elements
$U^{IJ}_{\mu\nu}$	nuclear attraction matrix elements
$h^{IJ}_{1\mu\nu}$	one-electron matrix elements
$\langle\mu\gamma\|\nu\delta\rangle$, $\langle\phi^I_\mu\phi^K_\gamma\|\phi^J_\nu\phi^L_\delta\rangle$	two-electron integrals
$O^{IJ}_{\mu\nu}(\mathbf{r})$	overlap distribution or differential overlap
ε^I_α	on-site energies
$t^{IJ}_{\alpha\beta}$, $\beta^{IJ}_{\alpha\beta}$	hopping or resonance integrals
$C_{LL'L''}$	Gaunt coefficients
$B_{JL',IL}$	structure constants
R_{MT}	muffin-tin radius

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Acronyms

Quantum chemistry

CASSCF	complete active space self-consistent field
CI	configuration interaction
CC	coupled clusters
ECP	effective core potential
HF	Hartree–Fock
RPA	random phase approximation
MCSCF	multi-configuration self-consistent field
MRCI	multi-reference configuration interaction
MP	Møller–Plesset perturbation theory
S,D,T,Q	single, double, triple, and quadruple excitations
SCF	self-consistent field

Density functional theory

DFT	density functional theory
DFPT	density functional perturbation theory
DMFT	dynamical mean-field theory
EXX	exact exchange
GGA	generalized gradient approximation
KS	Kohn–Sham
LDA	local density approximation
LSDA	local spin density approximation
MBPT	many-body perturbation theory
OEP	optimized effective potential
SIC	self-interaction correction
TFD	Thomas–Fermi–Dirac
WDA	weighted density approximation
XC	exchange-correlation

Plane wave and related methods

AE	all-electron
BZ	Brillouin zone
FFT	fast Fourier transform

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KB	Kleinman–Bylander
NLCC	non-linear core corrections
OPW	orthogonalized plane waves
PAW	projected augmented waves
PBC	periodic boundary conditions
PPW	pseudopotential plane wave
PS	pseudopotential
PW	plane waves
US	ultrasoft

Atom-centered methods

AO	atomic orbital
BSSE	basis set superposition error
CGTO	contracted Gaussian-type orbitals
GTO	Gaussian-type orbitals
HOMO	highest occupied molecular orbital
LCAO	linear combination of atomic orbitals
LUMO	lowest unoccupied molecular orbital
MO	molecular orbital
PGTO	primitive Gaussian-type orbitals
STO	Slater-type orbitals
SZ,DZ,DZP,TZP, etc.	single-zeta, double-zeta+polarization, etc.

Augmentation and related methods

APW	augmented plane waves
ASA	atomic sphere approximation
FP	full-potential
KKR	Korringa–Kohn–Rostoker
LAPW	linearized augmented plane waves
LCMTO	linear combination of muffin-tin orbitals
LMTO	linear muffin-tin orbitals
MT	muffin-tin
MTA	muffin-tin approximation
MTO	muffin-tin orbitals

Simplified methods

AM1	Austin model 1
CNDO	complete neglect of differential overlap
EAM	embedded atom model
INDO	intermediate neglect of differential overlap
MINDO	modified intermediate neglect of differential overlap
MNDO	modified neglect of differential overlap
NDDO	neglect of diatomic differential overlap
PM3	parametric model 3
QM – MM	quantum mechanics – molecular mechanics
SCCT	self-consistent charge transfer

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SCTB	self-consistent tight-binding
TB	tight-binding
ZDO	zero differential overlap

***Ab initio* molecular dynamics**

BOMD	Born–Oppenheimer molecular dynamics
CPMD	Car–Parrinello molecular dynamics
DFMD	density functional molecular dynamics
DKSO	dynamical Kohn–Sham orbitals

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