1 *THE* citation

- Roberto Car and Michele Parrinello, *Unified Approach for Molecular Dynamics and Density-Functional Theory*, [27]

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2 Books

2.1 DFT – particularly recommended

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  Note: Very good, yet theoretical; see also the upcoming revised edition

- R. M. Martin, *Electronic Structure: Basic Theory and Practical Methods*, [144]

  Note: for additional information, errata, web resources etc. see `http://electronicstructure.org/`

2.2 (Classical) Molecular dynamics – particularly recommended

- M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, [4]

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- D. Frenkel and B. Smit, *Understanding Molecular Simulation – From Algorithms to Applications*, [55]

2.3 Others

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- P. W. Atkins, *Molecular Quantum Mechanics*, [8]

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- G. Ciccotti, D. Frenkel and I. R. McDonald, *Simulation of Liquids and Solids*, [36]

- S. Goedecker, *Wavelets and their application for the solution of partial Differential equations in physics*, [61]

- H. Goldstein, C. P. Poole and J. L. Safko, *Classical Mechanics*, [69]

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- W. J. Hehre, L. Radom, P. v. R. Schleyer and J. A. Pople, *Ab Initio Molecular Orbital Theory*, [86]

- T. Helgaker, P. Jørgensen and J. Olsen, *Molecular Electronic Structure Theory*, [91]

- M. Kaupp and M. Bühl, V. G. Malkin, *Calculation of NMR and EPR Parameters*, [120]

- A. Messiah, *Quantum Mechanics*, [153]

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- R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules*, [162]

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- D. J. Singh, *Planewaves, Pseudopotentials and the* LAPW *Method*, [204]

3 Reviews

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  Note: see `http://www.theochem.rub.de/go/cprev.html`

- S. Baroni, S. de Gironcoli, A. Dal Corso and P. Giannozzi, [11]

  `http://dx.doi.org/10.1103/RevModPhys.73.515`,

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- G. Galli and M. Parrinello, *Computer Simulations in Materials Science*, [58]

- M. J. Gillan, *Calculation of the vacancy formation energy in aluminium*, [60]

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- D. Marx and J. Hutter, *Ab Initio Molecular Dynamics: Theory and Implementation*, in *Modern Methods and Algorithms of Quantum Chemistry*, [145]

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- G. Pastore, E. Smargiassi and F. Buda, [170]

- M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias and J. D. Joannopoulos, *Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients*, [171]

  `http://dx.doi.org/10.1103/RevModPhys.64.1045`,

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- R. Resta, *Macroscopic polarization in crystalline dielectrics: the geometric phase approach*, [188]

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4 Codes

- J. Hutter *et al.*, CPMD, [47]

  http://www.cpmd.org/

  Note: Car-Parrinello Molecular Dynamics: An *Ab Initio* Electronic Structure and Molecular Dynamics Program; IBM Zurich Research Laboratory (1990-2006) and Max-Planck-Institut für Festkörperforschung (1997-2001); for downloads see http://www.cpmd.org/, URL = http://www.cpmd.org/

- CP2k *A General Program to Perform Molecular Dynamics Simulations*, [37]

  http://cp2k.berlios.de/

  Note: CP2k developers group under the terms of the GNU General Public License; see http://cp2k.berlios.de/in

- ABINIT, [1]

  http://www.abinit.org/

  Note: Ref. [73]; distributed under the terms of the GNU General Public License; see http://www.abinit.org/,

- CASTEP, [31]

  http://www.tcm.phy.cam.ac.uk/castep/

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- COSMO*logic* GmbH & Co. KG, Leverkusen and Germany, [121]

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- P. E. Blöchl, CP-PAW, [17]

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- W. F. van Gunsteren, S. R. Billeter, A. A. Eising, P. H. Hünenberger, P. Krüger, A. E. Mark, W. R. P. Scott and I. G. Tironi, *Biomolecular Simulation:* GROMOS96 *Manual and User Guide*, [229]

  Note: Molecular mechanics; BIOMOS b.v. ETH, Zürich 1996

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  Note: Ref. [**?**]; developed and distributed by Pacific Northwest National Laboratory, USA; see http://www.emsl.pnl.gov/docs/nwchem/,

- PINY, [181]

  http://homepages.nyu.edu/~mt33/PINY_MD/PINY.html

  Note: The PINY_MD(c) Simulation Package; Principle Authors: G. J. Martyna and M. E. Tuckerman; Other Authors: D. A. Yarne, S. O. Samuelson, A. L. Hughes, Y. Liu, Z. Zhu, M. Diraison, K. Pihakari; see Ref. [228] for the method; see http://homepages.nyu.edu/~mt33/PINY_MD/PINY.html,

- PWscf, [185]

  http://www.pwscf.org/

  Note: Plane-Wave Self-Consistent Field is a set of programs for electronic structure calculations within Density-Functional Theory and Density-Functional Perturbation Theory, using a Plane-Wave basis set and pseudopotentials; PWscf is released under the GNU General Public License; see http://www.pwscf.org/,

- S/PHI/nX (or SFHIngX), [196]

  Note: written by S. Boeck, J. Neugebauer *et al.*; see http://www.sfhingx.de/

- SIESTA, [197]

  http://www.uam.es/departamentos/ciencias/fismateriac/siesta/

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5 Articles

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- R. O. Jones and O. Gunnarsson, *The density functional formalism, its applications and prospects*, [119]

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5.2 CPMD — Methods

- G. Berghold, C.J. Mundy, A.H. Romero, J. Hutter and M. Parrinello, *General and efficient algorithms for obtaining maximally localized Wannier functions*, [14]

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- P. E. Blöchl, [18]

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- X. Gonze and R. Stumpf amd M. Scheffler, *Analysis of separable potentials*, [72]

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  Note: see `http://psi-k.dl.ac.uk/index.html?highlights` and `http://psi-k.dl.ac.uk/newsletters/News_16`

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- H. Hellmann, [93]

  Note: see equation (3b); note that Hellmann already connects the "Hellmann-Feynman theorem" to first-order perturbation theory for cases where it does not hold rigorously, for instance when the wavefunction used to evaluate the expectation value is not the exact one.

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