

fort.10, fort.11, fort.14, fort.15...



**A Celebratory Symposium on the occasion of
Mike Payne's 60th birthday**

Session 1: Fundamental Methods of Electronic Structure

Nicola Marzari, EPFL



1960

1960 was an outstanding year, declared by all of the major Port houses.

Now settled into glorious Vintage Port of the very highest quality.

A superb combination of lovely mature fruit with the elegance that only this length of time in bottle can give.

Prof Mike Payne FRS

- 1996 Maxwell Medal and Prize, awarded by the Institute of Physics
- 1998 Mott Lecture, awarded by the Institute of Physics.
- 1999 Citation Superstar of the U.K., awarded by the Institute for Scientific Information
- 2008 Elected Fellow of the Royal Society
- 2011 Elected Honorary Fellow of the Institute of Physics
- 2014 Swan Medal, awarded by the Institute of Physics

Prof Mike Payne FRS

- Michael Payne is an outstanding physicist whose work focuses on first principles total energy calculations. **Michael's computational techniques have revolutionised materials design and facilitated the industrial application of quantum mechanical simulations.** He is responsible for the widespread adoption of the total energy pseudopotential technique and is the original author of the CASTEP code.
- He has **developed robust, efficient minimisation techniques** — critical for the 'black box' implementation of pseudopotential calculations, making the methodology accessible to non-experts. Michael also contributed to the **development of optimal, minimal scaling algorithms** for the computationally intensive parts of the calculations.
- In addition, Michael was responsible for the **implementation of codes on parallel computers**, allowing the first fully optimised quantum mechanical calculations to be performed for systems containing hundreds of atoms.

Inelastic electron tunnelling spectroscopy

M C Payne and J C Inkson

Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

Received 4 February 1983

To derive the matrix element for the inelastic tunnelling process and hence the magnitude of the weighting function we need to know the following:

- (i) the electron wavefunction in the barrier;**
- (ii) the phonon modes of the barrier;**
- (iii) the electron-phonon coupling.**

Inelastic electron tunnelling spectroscopy

M C Payne and J C Inkson

Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

Received 4 February 1983

We use the results Of Chelikowsky and Schluter (1977) obtained by a
self-consistent pseudopotential calculation

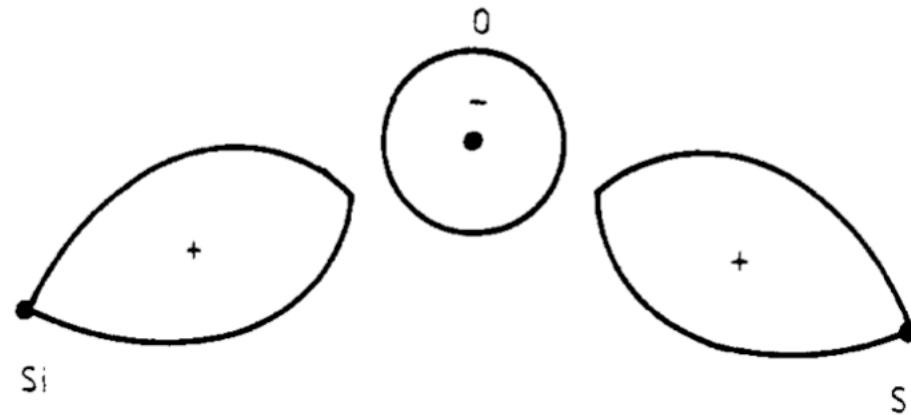


Figure 4. The basic orbital unit of the lowest three conduction bands. It contains 90% silicon sp^3 hybrids with 10% oxygen 2s in the antibonding configuration.

Molecular Dynamics and *ab Initio* Total Energy Calculations

In a recent Letter,¹ Car and Parrinello described a molecular-dynamics approach to total-energy calculations that allows global minimization of the total energy to be achieved with respect to both electronic and ionic coordinates. In this Comment, we shall briefly describe a number of modifications we have made to Car and Parrinello's method that can significantly increase the speed of the computation.

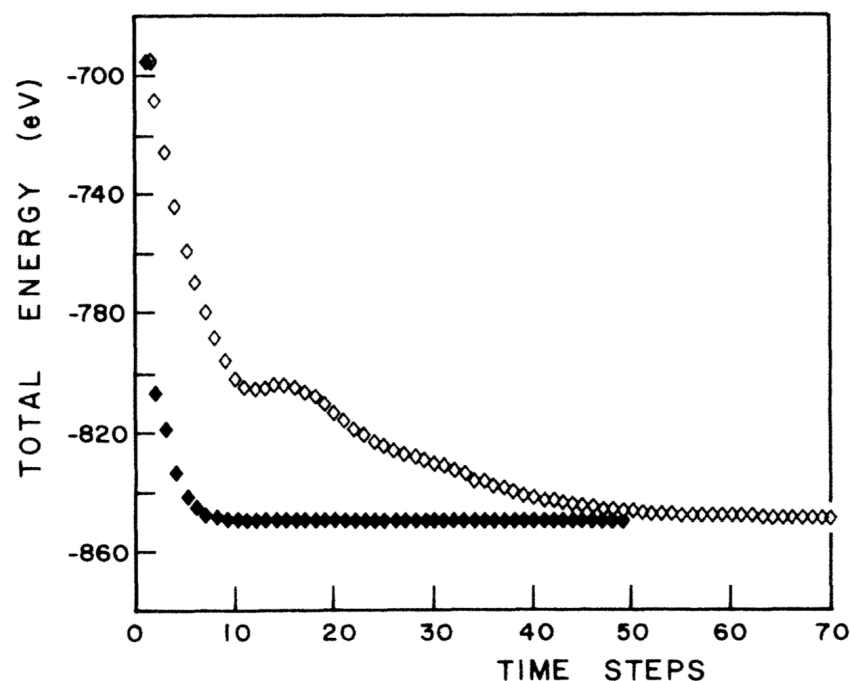


FIG. 1. Evolution of the total energy for an eight-atom cell of germanium in the diamond structure.

M. C. Payne and J. D. Joannopoulos
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

D. C. Allan and M. P. Teter
Corning Glass Works
Corning, New York 14831

David H. Vanderbilt
Harvard University
Cambridge, Massachusetts 02138

***Ab Initio* Determination of the Structure of a Grain Boundary by Simulated Quenching**

M. C. Payne,^(a) P. D. Bristowe, and J. D. Joannopoulos

Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

(Received 5 January 1987)

Results of the first completely *ab initio* investigation of the microscopic structure of a grain boundary in a semiconductor are presented. By use of the molecular-dynamics–simulated annealing method for performing total-energy calculations within the local-density–functional and pseudopotential approximations, the $\Sigma=5$ (001) twist boundary in germanium is studied. A number of rotation-and-translation states are investigated leading to a prediction for the structure of this geometry. Evidence for the possible presence of novel defects and glasslike tunneling-mode states at grain boundaries is presented.

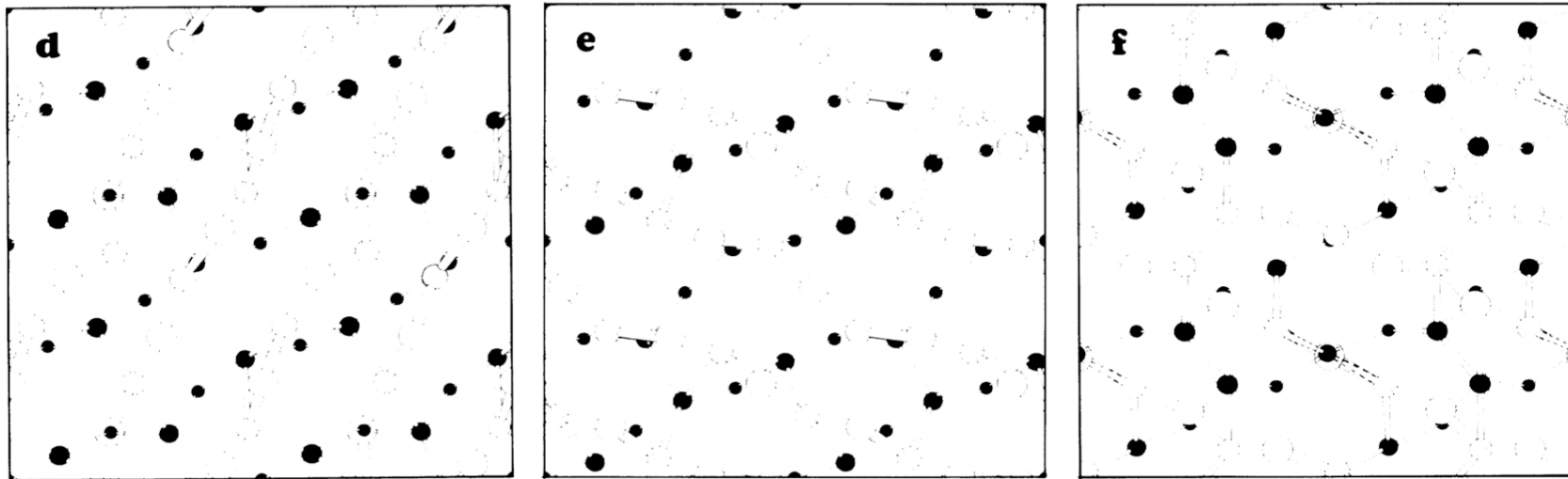


FIG. 1. Atomic positions in planes normal to the (001) direction for two layers above (open circles) and below (filled circles) a twist-grain boundary in germanium. (a) Unrelaxed $\Sigma 5$ CSL; a typical unit cell is indicated. (b) Relaxed $\Sigma 5$ CSL. (c) Unrelaxed $\Sigma 5 \frac{1}{20} \langle 210 \rangle$ state. (d) Relaxed $\Sigma 5 \frac{1}{20} \langle 210 \rangle$ state. (e) Relaxed $\Sigma 5^*$ CSL. (f) Relaxed $\Sigma 5^* \frac{1}{10} \langle 210 \rangle$ state.

Electrostatic and electrochemical potentials in quantum transport

M C Payne

Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

Received 23 January 1989, in final form 13 March 1989

Abstract. Self-consistent solutions for the electrostatic and electrochemical potentials are presented for idealised systems of perfect conductors connected to a perfect battery. A variety of phenomena are observed including electron transport against the gradient of the electrochemical potential.

$$G = \frac{2e^2}{\pi\hbar} \left(\sum_i T_i \right) \left(\sum_i v_i^{-1} \right) / \sum_i v_i^{-1} (1 + R_i - T_i)$$

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Electrostatic and electrochemical potentials in quantum transport

M C Payne

Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

Received 23 January 1989, in final form 13 March 1989



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The NEGF Approach to Nano-Device Simulation

by [Supriyo Datta](#)

The non-equilibrium Greens function (NEGF) formalism provides a powerful conceptual and computational framework for treating quantum transport in nanodevices. It goes beyond the Landauer approach for ballistic, non-interacting electronics to include inelastic scattering and strong correlation effects at an atomistic level.

Solution of Schrödinger's equation for large systems

Michael P. Teter

*Applied Process Research, Corning Glass Works, Corning, New York 14831
and Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853-2501*

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Douglas C. Allan

Applied Process Research, Corning Glass Works, Corning, New York 14831

(Received 24 April 1989; revised manuscript received 7 August 1989)

Iterative diagonalization of the Hamiltonian matrix is required to solve very large electronic-structure problems. Present algorithms are limited in their convergence rates at low wave numbers by stability problems associated with large changes in the Hartree potential, and at high wave numbers with large changes in the kinetic energy. A new method is described which includes the effect of density changes on the potentials and properly scales the changes in kinetic energy. The use of this method has increased the rate of convergence by over an order of magnitude for large problems.

1) The gradient

$$\nabla E_{Gn} = \frac{\partial E}{\partial C_{Gn}^*} + \sum_m \sum_{G'} \frac{\partial^2 E}{\partial C_{Gn}^* \partial C_{G'm}} \delta C_{G'm}$$

1) The gradient

$$\nabla E_{Gn} = \frac{\partial E}{\partial \mathbf{C}_{Gn}^*} + \sum_m \sum_{G'} \frac{\partial^2 E}{\partial \mathbf{C}_{Gn}^* \partial \mathbf{C}_{G'm}} \delta \mathbf{C}_{G'm}$$

2) The band-by-band minimization

$$\mathbf{C}_m^{n+1} = \mathbf{C}_m^n \cos \theta + \mathbf{D}^n \sin \theta$$

1) The gradient

$$\nabla E_{Gn} = \frac{\partial E}{\partial C_{Gn}^*} + \sum_m \sum_{G'} \frac{\partial^2 E}{\partial C_{Gn}^* \partial C_{G'm}} \delta C_{G'm}$$

2) The band-by-band minimization

$$\mathbf{C}_m^{n+1} = \mathbf{C}_m^n \cos \theta + \mathbf{D}^n \sin \theta$$

3) The pre-conditioning

$$K_{GG'} = \delta_{GG'} \frac{27 + 18x + 12x^2 + 8x^3}{27 + 18x + 12x^2 + 8x^3 + 16x^4}$$

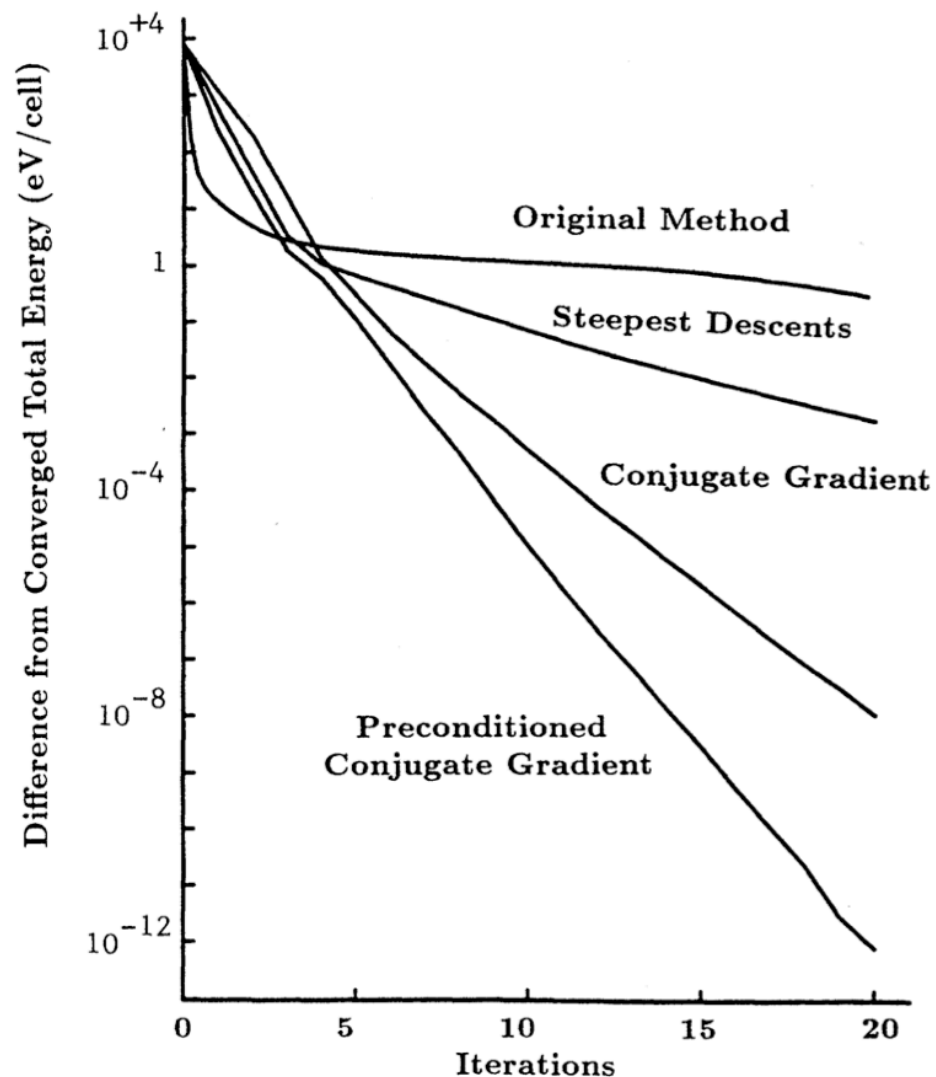


FIG. 2. The total energy error in eV/(unit cell) of an 8-atom silicon cube with a 16-hartree kinetic-energy cutoff vs iteration number for various methods. The scales are different for the different methods. The number of iterations of the original Williams-Soler method has been divided by 5 to allow comparison at the same level of computational effort.

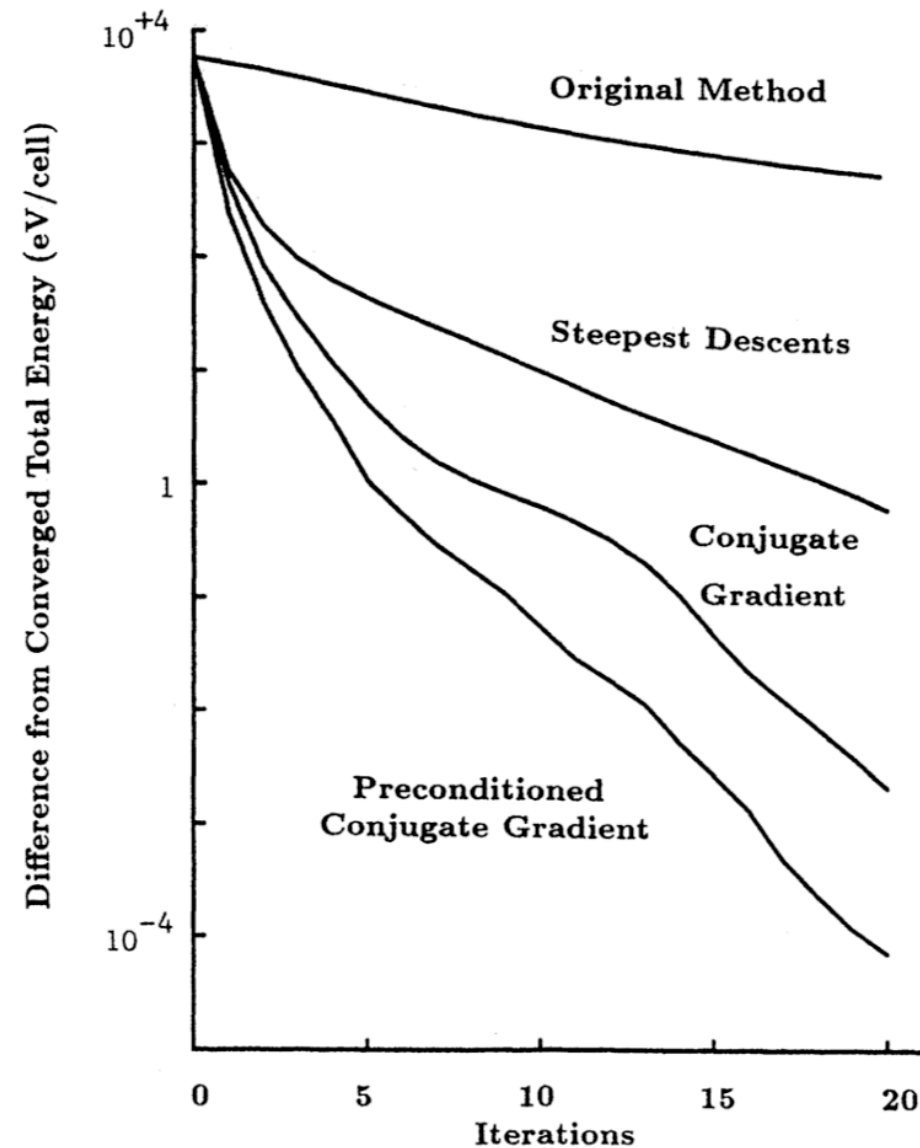


FIG. 3. The total-energy error in eV of a row of 12 silicon unit cells with a 4-hartree kinetic-energy cutoff vs iteration number for various methods. The methods are scaled as in Fig. 2.

Real-space implementation of nonlocal pseudopotentials for first-principles total-energy calculations

R. D. King-Smith,* M. C. Payne, and J. S. Lin

Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, England

(Received 13 May 1991)

We present a real-space method for performing the operations that involve the nonlocal parts of the Kohn-Sham Hamiltonian in a first-principles plane-wave total-energy calculation. In contrast to the conventional reciprocal-space formulation, where the number of operations required to compute the nonlocal contributions to the energies, forces, and stresses scales as the cube of the system size, the numerical work to compute these quantities with our real-space algorithm scales as the square of the number of atoms in the unit cell. The scheme, which can be applied to any potential expressible as a sum of separable terms, uses an approximate method to project the nonlocal potential on the core region of each atom. Errors introduced in the projection step are extremely well controlled and will not be a cause of problems in practical calculations. We have implemented the method in a conjugate-gradient total-energy program and, for illustrative purposes, demonstrate that the method produces excellent results on a two-atom cell of silicon.

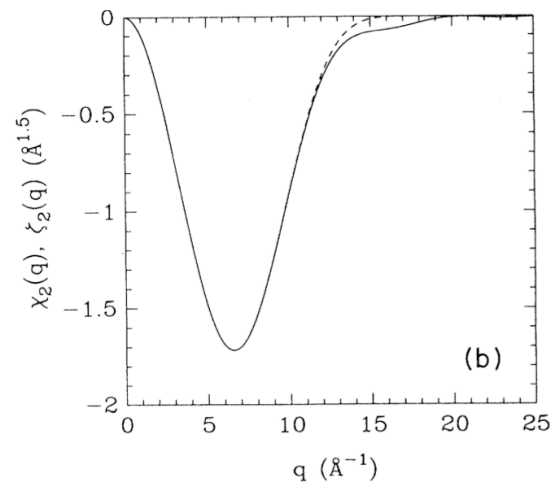
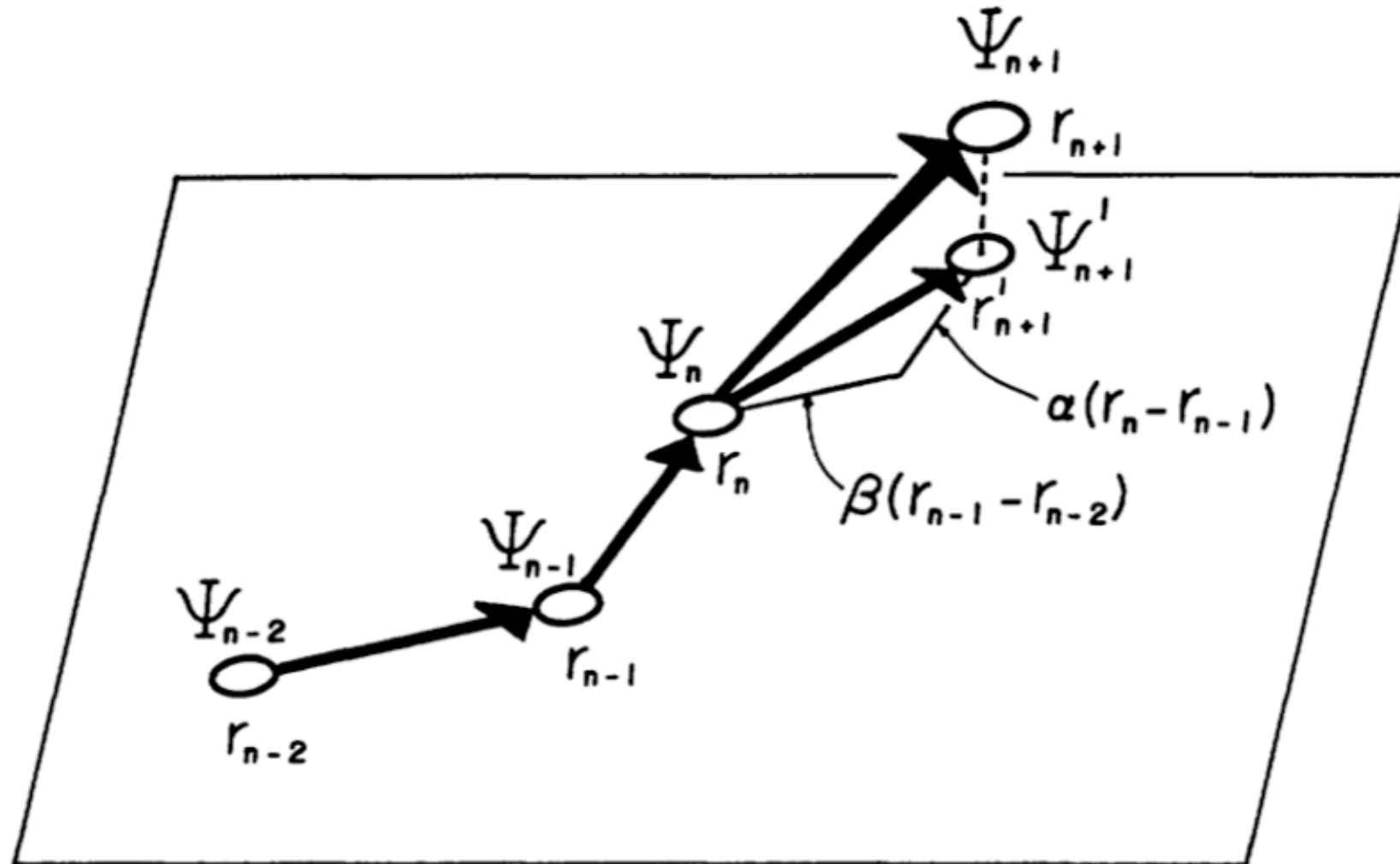


TABLE I. Comparison of nonlocal energies and forces for a two-atom cell of silicon calculated in real and reciprocal space using a conjugate-gradient total-energy program.

	Reciprocal space	Real space
Energy (eV)	-10.685 519 7	-10.685 513 9
Forces (eV/\text{\AA}) atom no. 1		
x	1.290 944	1.290 895
y	1.290 942	1.290 892
z	1.290 944	1.290 894
Forces (eV/\text{\AA}) atom no. 2		
x	-1.290 992	-1.291 024
y	-1.290 990	-1.291 022
z	-1.290 991	-1.291 024

***Ab initio* molecular-dynamics techniques extended to large-length-scale systems**

***Ab Initio* Molecular Dynamics: Analytically Continued Energy Functionals and Insights into Iterative Solutions**

T. A. Arias,⁽¹⁾ M. C. Payne,⁽²⁾ and J. D. Joannopoulos⁽¹⁾

⁽¹⁾*Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

⁽²⁾*Cavendish Laboratory, Madingley Road, Cambridge, CB30HE, United Kingdom*

(Received 26 May 1992)

We present a new method for performing finite-temperature *ab initio* total-energy calculations at long length scales, which we demonstrate with a dynamics calculation of 50-Å-long phonon modes in silicon. The method involves *both* a prescription for the analytic continuation of traditional fermionic energy functionals into the space of nonorthonormal single-particle orbitals (speeding convergence to the minimum) *and* insights into the common computational physics problem of solving by iterative refinement for the state of a complex system as a function of a continuous external parameter.

$$\frac{\partial E}{\partial \phi_k^\dagger} = A_k^\dagger F_k \hat{P}_k \hat{H}_{\text{LDA}} \psi_k - Q \{ V_k^\dagger [H_k, F_k] V_k \} V_k^\dagger \psi_k, \quad (7)$$

$$\frac{\partial E}{\partial [B_k^*]_{nm}} = - (R \{ [H_k, F_k] \})_{nm},$$

where F_k is a diagonal matrix loaded with the filling factors for each band n , \hat{P}_k is the projection operator

$$\hat{P}_k = \left[1 - \sum_n |\psi_{nk}\rangle \langle \psi_{nk}| \right], \quad (8)$$

Iterative minimization techniques for *ab initio* total-energy calculations: molecular dynamics and conjugate gradients

M. C. Payne

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Applied Process Research, Corning Incorporated, Corning, New York 14831

T. A. Arias and J. D. Joannopoulos

Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

This article describes recent technical developments that have made the total-energy pseudopotential the most powerful *ab initio* quantum-mechanical modeling method presently available. In addition to presenting technical details of the pseudopotential method, the article aims to heighten awareness of the capabilities of the method in order to stimulate its application to as wide a range of problems in as many scientific disciplines as possible.

Iterative minimization techniques for *ab initio* total-energy calculations: molecular dynamics and conjugate gradients

M. C. Payne

Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, United Kingdom

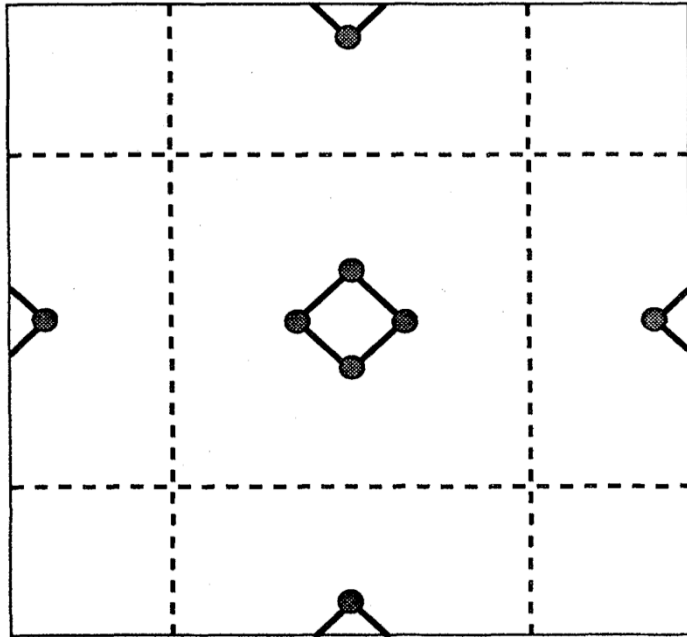


FIG. 4. Schematic illustration of a supercell geometry for a molecule. Same convention as in Fig. 2.

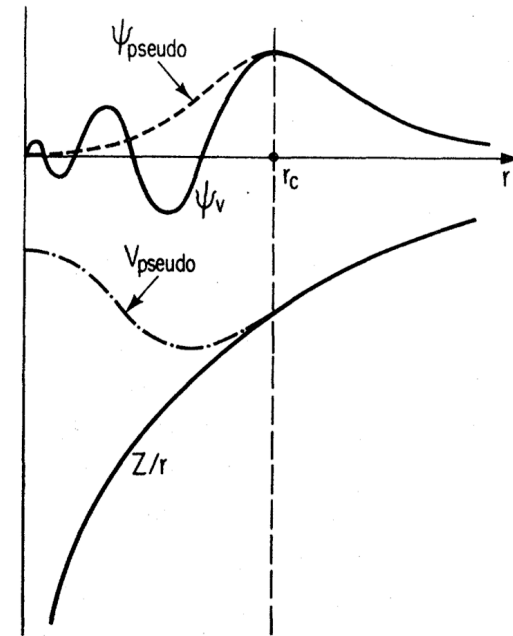


FIG. 5. Schematic illustration of all-electron (solid lines) and pseudoelectron (dashed lines) potentials and their corresponding wave functions. The radius at which all-electron and pseudoelectron values match is designated r_c .

Iterative minimization techniques for *ab initio* total-energy calculations: molecular dynamics and conjugate gradients

M. C. Payne

Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, United Kingdom

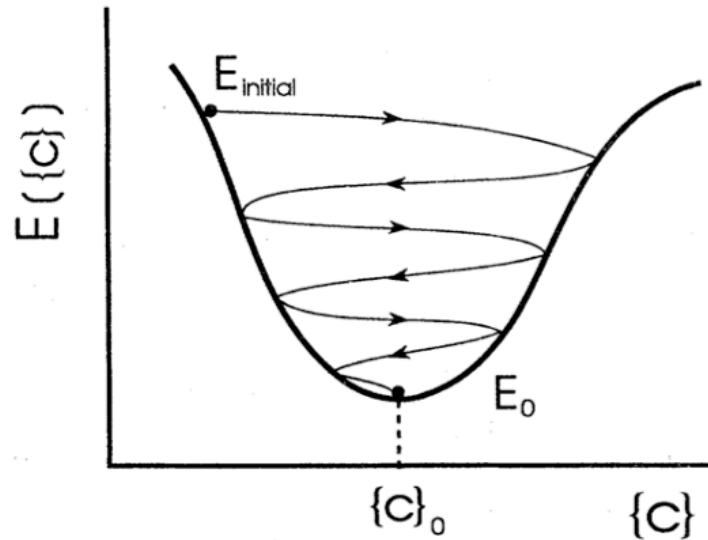


FIG. 9. Schematic representation of the damping of wave-function coefficients $\{c\}$ and the evolution of the Kohn-Sham energy functional $E[\{c\}]$ to its ground-state value E_0 .

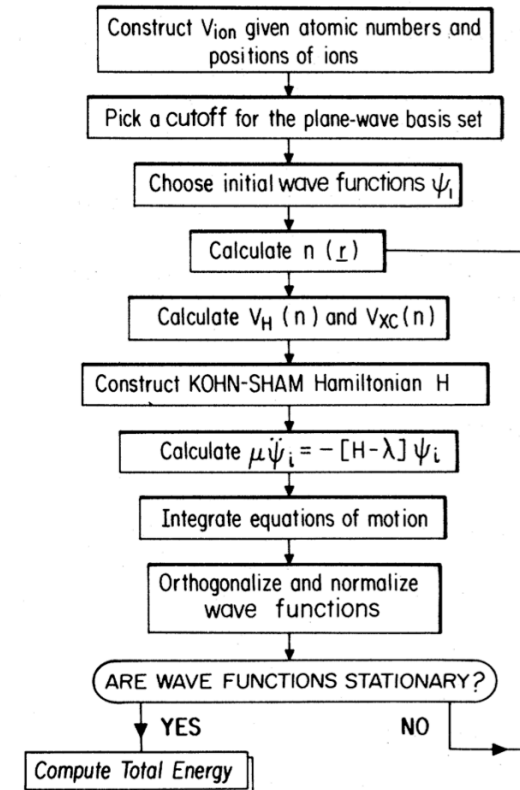


FIG. 11. Flow chart describing the computational procedure for the calculation of the total energy of a solid with molecular dynamics.

Iterative minimization techniques for *ab initio* total-energy calculations: molecular dynamics and conjugate gradients

M. C. Payne

Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, United Kingdom

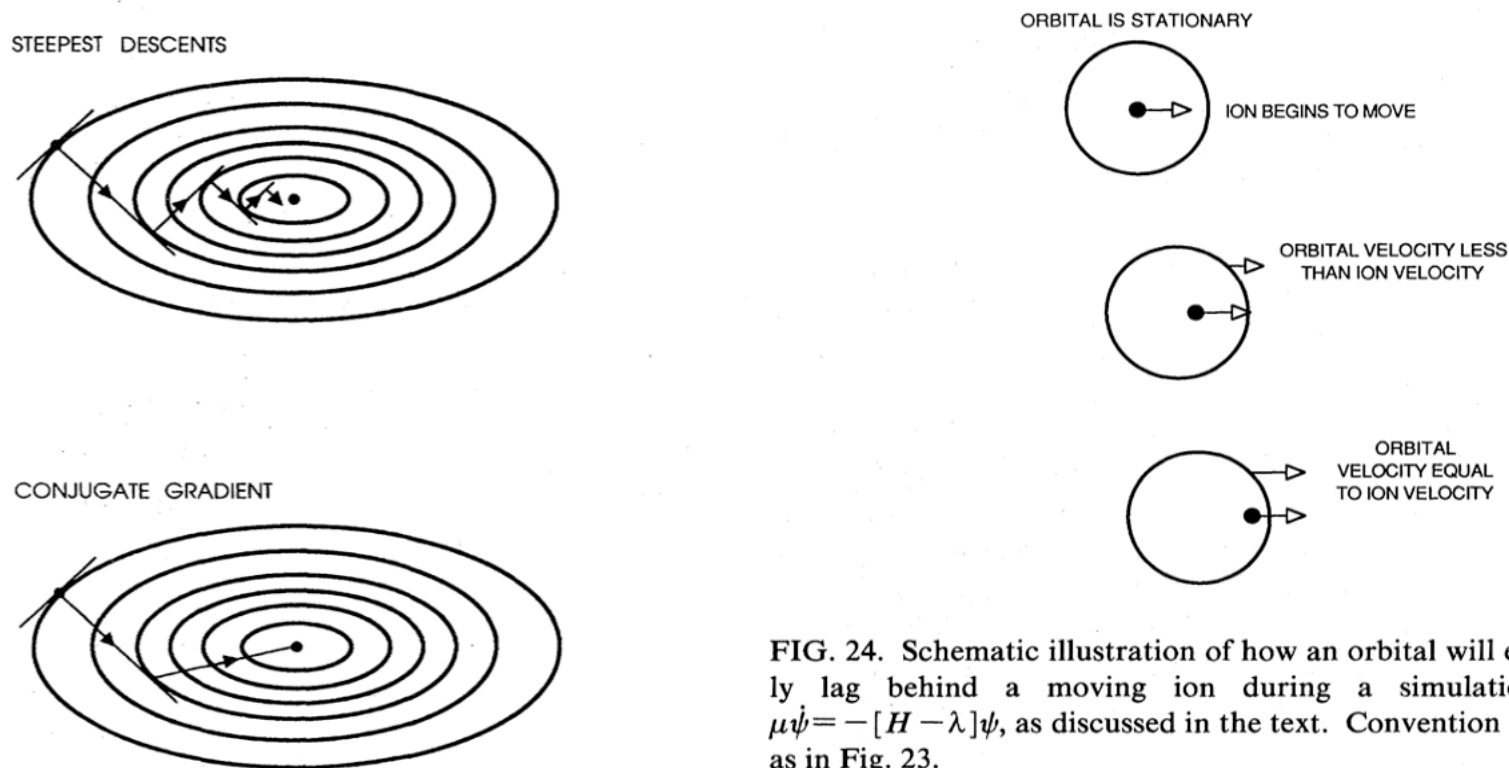


FIG. 24. Schematic illustration of how an orbital will eventually lag behind a moving ion during a simulation with $\mu\dot{\psi} = -[H - \lambda]\psi$, as discussed in the text. Convention the same as in Fig. 23.

From: 19512::ADV "Dr A DeVita" 4-JUN-1992 00:06:33.78

**To: @[ADV.OHNOPLEASEDONT.EVIL_CHAPS.VERY_BADGUYS.UGLYPUNKS]
LARDYPIG**

Subj: dovunque tu sii

From: 19512::ADV "Dr A DeVita" 4-JUN-1992 00:06:33.78

**To: @[ADV.OHNOPLEASEDONT.EVIL_CHAPS.VERY_BADGUYS.UGLYPUNKS]
LARDYPIG**

Subj: dovunque tu sii

**allora, juju, guarda che ho beccato mike payne a london, che aveva un invited, e
gli ho parlato di un mio amico obeso, e che puo' essere che gli serva in tempi brevi
un aiuto furbo da lui per stendere una domanda circostanziata per chiedere soldi
a entita' europofile per far phd a cambridge, e che sei genio e gli conviene.**

[...]

zio fa quel che puo', ciccionastro had better clarify, quel porcilante.

Date: Thu, 18 Jun 92 08:35:21 BST

From: MCP1@PHOENIX.CAMBRIDGE.AC.UK

To: marzari@tsmi19.sissa.it

Subject: EEC application

Message-ID: <A5DC3CDC0B74C060@UK.AC.CAMBRIDGE.PHOENIX>

Dear Nicola,

This is just to confirm that I have received your e-mail message which I am about to read. I shall get on with the relevant pieces of the application as immediately.

I very much hope that this application is successful and that you are able to come and work here.

Yours, Mike Payne.

Date: Thu, 18 Jun 92 09:09:55 BST

From: MCP1@PHOENIX.CAMBRIDGE.AC.UK

To: marzari@tsmi19.sissa.it

Subject: EEC application 2

Message-ID: <A5DC449558050670@UK.AC.CAMBRIDGE.PHOENIX>

Dear Nicola,

I hope that a project initially focussed on the supermodulus effect would be acceptable to you [...]

I am sure however that a continual exchange of e-mail will sort out most of the difficulties so please contact me whenever you come across any problems. I shall set a deadline of midday saturday to send you by e-mail all the things to be completed on the application forms. Independently I shall arrange for the sections to be written by the head of the host institution to be done here using the forms from the mail Sandro sends. **Can I just confirm that you will send me everything apart from these so that I can put the whole application together, make copies, and send them off next week. They will be sent by express mail no later than friday next week to guarantee arrival in Brussels by the deadline.**

If you see any problems with this please let me know, Mike.

Date: Fri, 26 Jun 92 20:25:56 BST

From: MCP1@PHOENIX.CAMBRIDGE.AC.UK

To: marzari@tsmi19.sissa.it

Subject: application

Message-ID: <A5E6EA9D5BBE6640@UK.AC.CAMBRIDGE.PHOENIX>

Dear Nicola,

Dont worry about the problems which as you say were out of your hands.

I am presently typing the whole thing onto the forms - the slight worry is that I am not going to be able to get copies of your articles and I suppose that something has to be done about your signature - I shall do my best although the bigger problem is the lack of a home institution stamp - I guess we have to hope that this is no great deal.

I better get back to the type writer - it is going to be a long night!

Mike.

From: MCP1@PHOENIX.CAMBRIDGE.AC.UK

To: marzari@tsml9.sissa.it

CC: adv@VMSFE.RUTHERFORD.AC.UK

Subject: EEC

Message-ID: <A67467EED2C4A430@UK.AC.CAMBRIDGE.PHOENIX>

Dear Nicola and Sandro,

A fat envelope from the EEC has just arrived saying that we have got the Bursary (actually it does not say that we have but gives every indication that we get money by signing forms and returning them to Bruxelles!) So, Nicola, should I go ahead and start sorting things out this end - if you wish to take up the bursary here you shall have to make a formal application to become a graduate at the University and I should do a few things to smooth the way first so let me know if we are definitely going ahead.

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CC: adv@VMSFE.RUTHERFORD.AC.UK

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Yippppeeeeeeee, I will have to become SLIGHTLY less critical of the EEC now!

Mike.

COMPUTATIONAL SCIENCE IN THE EARLY '90s

[illegible]

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INCLUDE 'param.inc'
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C
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CASTEP
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Cambridge Serial Total Energy Package
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Cambridge 1991
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C=====
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THIS IS A MODIFIED VERSION OF MC PAYNE'S CONJUGATE GRADIENT PROGRAM
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EFFORTS OF FOLLOWING COLLABORATORS WHO TOOK PART IN THE
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C
```

```
DEVELOPMENT OF THIS PACKAGE SHOULD BE MENTIONED :
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C
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LATE XUDONG WENG, VICTOR MILMAN, GRAHAM FRANCIS, UWE BERTRAM,
```

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C
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```
BJORK HAMMER ET AL.
```

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-
```

(A full copy of this manual--not to be printed---can be found in
/u/tcml/ftp/pub/castep/manual.txt.Z)

CASTEP / CETEP 1992

Cambridge Serial Total Energy Package and
Cambridge and Edinburgh Total Energy Package

Written by M.C.Payne and further modified by a number of collaborators
(late X.Weng, B.Hammer, G.Francis, I.Stich, U.Bertram, A.de Vita, J.S.Lin,
A.Qteish).

Current maintenance and subsequent changes are due to V.Milman.

Enquiries to: VYM10@uk.ac.cam.phx or
MILMAN@UK.AC.CAMBRIDGE.WEST.PHYSICS.

CONTENTS

1. INTRODUCTION
2. LIST OF SUBROUTINES
- 2.1 ESSENTIAL CASTEP
- 2.2 SYMMETRY ANALYSIS
3. STRUCTURE OF CASTEP
4. EXTERNAL FILES NEEDED FOR CASTEP
5. SYMMETRIZATION OF CHARGE DENSITY
6. BAND STRUCTURE CALCULATION
7. CONSTRAINED IONIC RELAXATION

- APPENDICES:
1. Example of jobfile to run CASTEP on VAX
 2. param.inc file to be included in the CGION
 3. File fort.14 - control parameters (8 atoms Si)
 4. File fort.15 - structural parameters, 8-atoms Si
 5. fort.3 generated by RUN290 code for 8 atoms Si
 6. Example of .com file to run symmetry package on VAX
 7. Eigenvalues for Si compared to other LDA
 8. Output for Si 8 atoms with 1 and 4 k-points
 9. CASTEP library contents for RS6000
 10. Estimated timings for CASTEP
 11. Specifications of CASTEP subroutines (version 2.1)
 12. Specifications of symmetry analysis subroutines (version 1.1)

1. INTRODUCTION

The CASTEP package contains routines to enable electronic relaxation to ground state for metals, insulators, or semiconductors. It calculates forces acting on atoms and stress on unit cell and allows ionic relaxation with the search of equilibrium structure. Non-orthorombic unit cells can be used with different kinds of atoms. Molecular dynamics simulations are possible. The electronic relaxation is achieved by minimization of the total energy with respect to wave functions defined on a plane wave basis set. Electron-ion interaction is described by ionic pseudopotential which can be either local or nonlocal. Nonlocal pseudopotential should be in a Kleinman-Bylander form. Corresponding projectors are calculated either in reciprocal (CASTEP) or in real space (CASTEP and CETEP) [1,2].

Main limitations : all LDA problems like energy gap in semiconductors etc.; absence of spin-orbit term (CASTEP is based on LDA rather than LSDA); big basis set required for transition metals and for elements with localised potentials (O,C,Cl etc.). CASTEP uses plane wave basis set

expansion of wave functions, charge density and potential so for the above mentioned elements it is less efficient as more basis states are required. The package is nonrelativistic.

The structure of the program is almost totally determined by the use of fast Fourier transforms. It uses also special K-points sampling for integration over the Brillouin zone. For metallic systems CASTEP introduces partial occupancies for levels close to the Fermi energy [3].

There are certain differences between CASTEP and its parallel version, CETEP, which are described later. The description given below refers to CASTEP only. CETEP is implemented on Meiko i860 machine with 64 nodes and on Intel i860a hypercube [4].

The 1.1 version uses only reciprocal space representation of the nonlocal pseudopotential. The 2.1 version has an option of using the real space method which is preferable for large systems. Description of the method is given in [5].

NOTE. These two versions are not compatible with the exception of few simplest routine. Extensive clearing work has been done to remove obsolete variables in 2.1 version, but now mixing of source files from these versions is prohibited.

- [1] M.P. Teter, M.C. Payne, and D.C. Allan, Phys. Rev. B40, 12255 (1989).
- [2] M.C. Payne, M.P. Teter, D.C. Allan, and J.D.Joannopoulos, in press.
- [3] C-L Fu and K-M Ho, Phys. Rev. B28, 5480 (1983).
- [4] L J Clarke, I Stich, M C Payne, Comp. Phys. Comm (in press).
- [5] R D King-Smith, M C Payne, J S Lin, Phys. Rev. B44, 13063 (1991).

2. LIST OF SUBROUTINES

2.1. ESSENTIAL CASTEP

CGION	main program of CASTEP
BASTR	calculates the set of basis vectors in reciprocal space
BMDTR	integrates the equations of motion for the size of unit cell
CHSP	constructs the electronic charge density
CLOCK	machine-dependent call of timer
CONGRA	conjugate gradient method for total energy minimisation with regard to electronic band coefficients
CONGRABS	calculates the band structure for given charge density
CONSTR	user-supplied routine for constrained minimisation
EFERMI	calculates the Fermi energy and occupation numbers
EWALTR	calculates Ewald energy and contributions to ionic forces and stress
FDIRTR	calculates the Hartree potential
FEICTR	calculates the stress which results from the electron-ion energy
FELITR	calculates the Hellmann-Feynman forces exerted on the ions
FEXCTR	calculates the exchange-correlation potential and corresponding contribution to stress
FFT3D	three dimensional fast Fourier transform
FORSYM	symmetrizes forces on ions calculated by summing over special points
FSTFTR	calculates structure factor on the grid of reciprocal vectors
FVPTR	calculates local pseudopotential on the grid of reciprocal vectors
GENBTR	initialises indexing system for plane waves
PHASGR	calculates phase factors for nonlocal components
SETVG	calculates nonlocal pseudopotential on the grid of reciprocal vectors
VNLWAV	calculates action of nonlocal pseudopotential on specific wavefunction
FNLFOR	calculates contribution to the Hellman-Feynman force from nonlocal potential
FSIGNL	calculates contribution to the stress from nonlocal potential
ORSP	orthonormalizes wavefunctions
REASSN	reassigns the wave function component for the case of re-

Year 1991

5th Total Energy and Forces Meeting



International Atomic Energy Agency



United Nations Educational, Scientific and Cultural Organization

International Centre for Theoretical Physics

News from ICTP

No. 42/43
January/February 1991

Year 1991

5th Total Energy and Forces Meeting



- Quantum Monte Carlo studies of materials
- Dielectric response and quasiparticle energies in Ni
- Lattice dynamics and instabilities in high T_c superconductors
- Localization in self-interaction corrected DFT
- Ab-initio calculations of free energies in real materials
- Polarization in ferroelectric BeO



No. 42/43
January/February 1991

From mcpl@phy.cam.ac.uk Thu Apr 4 06:17:13 1996

Date: Thu, 4 Apr 96 12:17 WET DST

From: mcpl@phy.cam.ac.uk (Mike Payne)

To: dhv@physics.rutgers.edu, marzari@physics.rutgers.edu

Subject: Thesis

Status: RO

Dear Nicola,

I gather that David is concerned that you finish the thesis and really wants everything done by 1st May. [...]

If we are to meet the 1st May deadline you must immediately give BOGS the **submission date - I would suggest nothing later than 26th April** - please copy this communication to me so I can hurry the process of appointing examiners. Then you and David should provisionally arrange the oral examination for 29th April - the other examiner to be chosen on the simple basis of who could make it that day. If reports are FAXED to me immediately after the viva I shall get the letter provisionally confirming the PhD to David on the 30th. **Please please agree to this timetable. [...]**

Yours, Mike.

Ensemble Density-Functional Theory for *Ab Initio* Molecular Dynamics of Metals and Finite-Temperature Insulators

Nicola Marzari,^{1,2} David Vanderbilt,¹ and M. C. Payne²

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(Received 7 March 1997)

A new method is presented for performing first-principles molecular-dynamics simulations of systems with variable occupancies. We adopt a matrix representation for the one-particle statistical operator $\hat{\Gamma}$ to introduce a “projected” free energy functional G that depends on the Kohn-Sham orbitals only and that is invariant under their unitary transformations. The Liouville equation $[\hat{\Gamma}, \hat{H}] = 0$ is always satisfied, guaranteeing a very efficient and robust variational minimization algorithm, that can also be extended to nonconventional entropic formulations. [S0031-9007(97)03810-6]

$$\begin{aligned}
 \frac{\delta A}{\delta f_{ji}} &= h_{ij} + \frac{\delta E_{\text{HXC}}}{\delta f_{ji}} - T \frac{\delta S}{\delta f_{ji}} - \mu \delta_{ij} \\
 &= h_{ij} + \int d\mathbf{r} \frac{\delta E_{\text{HXC}}}{\delta n(\mathbf{r})} \frac{\delta n(\mathbf{r})}{\delta f_{ji}} - T[s'(\mathbf{f})]_{ij} - \mu \delta_{ij} \\
 &= h_{ij} + V_{ij}^{[n]} - T[s'(\mathbf{f})]_{ij} - \mu \delta_{ij} = 0. \quad (4)
 \end{aligned}$$

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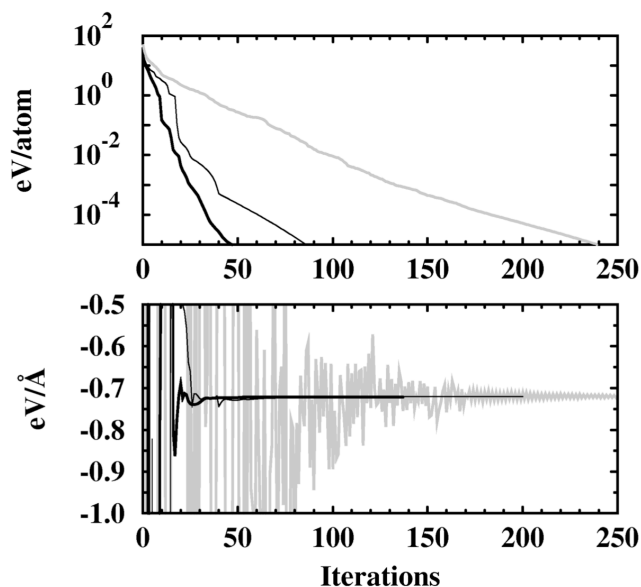


FIG. 1. Convergence of the total free energy (upper panel) and of the force on the surface atom (lower panel) in the 15-layer Al(110) slab. Grey line, ABV; thin (thick) solid line, ensemble DFT with two (four) iterations in the inner loop.

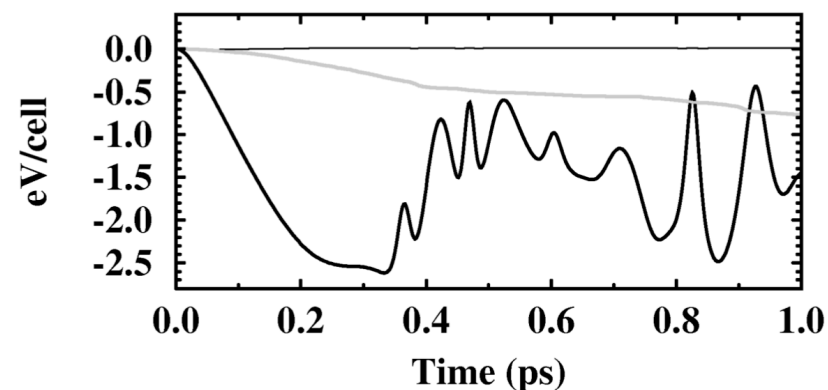


FIG. 2. Conservation of the constant of motion in a molecular-dynamics run for the 15-layer Al(110) slab. Bottom curve, electronic free energy; top two curves, same plus ionic kinetic energy (grey line, ABV; solid thin line, ensemble DFT with two iterations in the inner loop).

Happy Birthday Mike!

