DENSITY FUNCTIOAL THEORY

An introduction to DFT may be found in:

J.Weber, H.Huber and H.P.Weber,
Chimia vol 47, 57-59 (1993)
Computational Chemistry: All you ever wanted to know about density functional theory.

Best Wishes
Mark

I would be interested in the results of your query.
Jacek

Dr. Jacek Bieron
Internet: bieron@vuse.vanderbilt.edu

I, too, would like to see the sort of references you mention!
Please post a summary...
Irene Newhouse
NEELY@DUCVAX.AUBURN.EDU

Dear Andrew,
if you tell me what your surface mail address is, I'll send you some blurb about DMOL, which is BIOSYM's dft program.

Max

Andy,

I don't know much about QM/DFT. I would be interested in the information also. I would be interested to know what type of biological systems you plan to apply it to. (Just curious).

Thanks!
Mark
Cray Research, Inc.
Eagan, MN 55121

Internet: mwd@cray.com

Subject: Re: Density Function Theory
Me too, would you post good references? Thanks, Pat Hogue

Dear Andy,
Springer-Verlag published a couple of book on density functional methods. I attach the respective information for you. The book edited by J.K. Labanowski is in high demand and might be out of print (only few copies were available when I last looked into the sales figures). There have also been several contributions to Theor. Chim. Acta.

Sincerely yours,
Dr. Rainer Stumpe
Chemistry Editorial
Springer-Verlag
Tiergartenstr. 17
D-69121 Heidelberg
Phone: +49-(0)6221-48 73 10
Fax: +49-(0)6221-41 39 82
INTERNET:stumpe@spint.compuserve.com

LECTURE NOTES IN CHEMISTRY VOL. 50

D. MUKHERJEE, Calcutta, India (Ed.)
Aspects of Many-Body Effects in Molecules and Extended Systems

---

PROCEEDINGS OF THE WORKSHOP-CUM-SYMPOSIUM HELD IN CALCUTTA,

February 1-10, 1988
1989. VIII, 565 pp. Soft cover DM 128,-. ISBN 3-540- 50765-5
Contents:

- Separability in Many-Electron Problem;
- Size Extensivity and Size-Consistency.
- Many-Body Perturbation Theory and Coupled-Cluster Theory of Atomic and Molecular Electronic Structure.
- Propagators in Bound States and Resonances.
- Condensed Matter and Related Topics.
- Many- Body Methods in Dynamical Processes.
- Relativistic Methods with Applications.

- Group-Theoretic Techniques.
- Few-Body Methods, Large-N Expansion and Other Mathematical Topics.
- Densities and Density-Functionals.
- List of Participants.
- Subject Index.

This volume features invited lectures presented in the workshop-cum-symposium on aspects of many-body effects in molecules and extended systems, Calcutta, February 1 - 10, 1988. The organizers invited leading experts to present recent developments of many-body methods as applied to molecules and condensed systems. The panorama portrayed is quite broad, but by no means exhaustive. The emphasis is undoubtedly on a "molecular point of view".

U. HARMS, INDUSTRIEANLAGEN-BETRIEBSGESELLSCHAFT (IABG)

Ottobrunn, FRG (Ed.)

SUPERCOMPUTER AND CHEMISTRY

IABG Workshop 1989

1990. Approx. 150 pp. 46 figs. 38 tabs. Softcover DM 98,- ISBN 3-540-52915-2

This volume represents the contributions of the 1989 IABG workshop on supercomputers and chemistry.

>From the CONTENTS :

- Transputer Graphic Supercomputing MIMD Type Computers Drug Design Peptide and Protein Engineering Density Functional Calculations
- Computational Chemistry, Theoretical Chemistry, Drug Design, Protein Engineering, Super and Parallel Computing, Transputer

Applications

For industrial and academic researchers, research managers in industry and computer manufacturers and vendors in the above-mentioned fields

---

J.K. LABANOWSKI, OHIO SUPERCOMPUTER CENTER, COLUMBUS, OH; J.W.

Andzelm, Cray Research Inc., Eagan, MN (Eds.)

Density Functional Methods in Chemistry

1991. XII, 443 pp. 68 figs. Hardcover DM 128,- ISBN 3-540-97512-8

Predicting molecular structure and energy and explaining the nature of bonding are central goals in quantum chemistry. In this volume, which is based on a 1990 workshop at the Ohio Supercomputer Center, leading experts on the density functional (DF) method and its chemical applications demonstrate how their work contributes to these goals and has come into its own as an advanced method of computational chemistry. Density functional theory emerged as an alternative to the traditional ab initio and semiempirical approaches of quantum chemistry for studying the ground state properties of molecular systems. Advantages of the method are its high accuracy and efficiency, which make it particularly well suited for the realistic study of large molecular systems of practical importance. It describes with consistent reliability organic, in organic, metallic, and semiconductor systems consisting of elements throughout the periodic table. For these reasons, density functional methodology is used increasingly in pharmaceutical, agrochemical, and biotechnology research; materials and polymer science; catalysis, surface and solid state research; and electrochemistry and microelectro nics. The wealth of applications presented in this book will make it a valuable tool for researchers faced with a growing choice of software and theoretical approaches.

STRUCTURE AND BONDING VOLUME 80

Chemical Hardness

K. Sen, University of Hyderabad, India; D.M.P. Mingos, Imperial College of Science, Technology and Medicine, London, UK (Eds.)

With contributions by numerous experts
1993. Approx. 280 pp. 52 figs. Hardcover DM 228,- ISBN 3-540-56091-2

Contents:

- R.G. Pearson, Santa Barbara, CA: Chemical Hardness - An Historical Int roduction.
- P.K. Chattaraj, Karagpur, India; R.G. Parr, Chapel Hill, NC: Density Functional Theory of Chemical Hardness.
- J.L. Gazqu z, Mexico, Mexico: Hardness and Softness in Density Functional Theory.- L. Komorowski, Wroclaw, Poland: Har dness Indices for Free and Bonded Atoms.
- N.H. March, Oxford, UK: The GroundStat e Energy of Atomic and Molecular Ions and Its Variation with the Number of Elect rons.
- K. Sen, Hyderabad, India: Isoelectronic Changes in Energy, Electronegativ ity, and Hardness in Atoms via the Calculations of <r-1>.
- P. Politzer, J.S. Mur ray, M.E. Grice, New Orleans, LA: Charge Capacities and Shell Structures of Atoms.
- R. F. Nalewajski, Cracow, Poland: Hardness Based Molecular Charge Sensitivit ies and Their Use in the Theory of Chemical Reactivity.

- B.G. Baekelandt, R. A. Schoonheydt, W.J. Mortier, Leuven-Heverlee, Belgium: The EEM Approach to Chemica l Hardness in Molecules and Solids: Fundamentals and Applications.
- J.A. Alonso, L.C. Balbas, Valladolid, Spain: Hardness of Metallic Clusters.

Z. ZHOUR, P.K. CHATTARAJ, R.G. PARR, C. LEE

First-order gradient correction for the exchange-energy density functional for atoms
Theoretica Chimica Acta Volume 84 Number 3, p 237

P. POLITZER, J. M. SEMINARIO, M. C. CONCHA, J. S. MURRAY

Some applications of local density functional theory to the calculation of reaction energetics
Theoretica Chimica Acta Volume 85 Number 1-3, p 127

D. HEINEMANN, A. ROSEN

Basis-independent potential energy curves for the neutral diatomics of Li, Na and K evaluated by means of Hartree-Fock and different density functional potentials
Theoretica Chimica Acta Volume 85 Number 4, p 249

Here are a few references which contain systematic comparisons of various properties of small molecules by DFT and conventional ab initio (HF, MP2, QCI) as well as experiment. Some of the references therein are also useful along these lines. I hope you find them helpful.

B. G. Johnson, P. M. W. Gill and J. A. Pople, J. Chem. Phys. 98, 5612 (1993).
A. D. Becke, J. Chem. Phys. 98, 5648 (1993).
A. D. Becke, J. Chem. Phys. 97, 9173 (1992).
A. D. Becke, J. Chem. Phys. 96, 2155 (1992).
J. Andzelm and E. Wimmer, J. Chem. Phys. 96, 1280 (1992).

Benny Johnson
Department of Chemistry
Carnegie Mellon University

Message 39/53 from rec@ncifcrf.gov Aug 5 '93 at 12:04 (noon)
Reply-To: cachau@ncifcrf.gov

A good reference book is:

"Density Functional Methods in Chemistry"
Jan K. Labanowski & Jan W. Andzelm Ed.
Springer-Verlag Berlin ISBN 3-540-97512-8

We have made a systemmatic comparison of polarizabilities and
hyperpolarizabilities calculated at the HF level (with HONDO8),
with 2 different DFT programs (deMon and DMol), and with experiment.
The reference is ...

J. Guan, P. Duffy, J.T. Carter, D.P. Chong, K.C. Casida, M.E. Casida,
and M. Wrinn, J. Chem. Phys. 98 (1993) 4753.
``Comparison of local-density and Hartree-Fock calculations of
molecular polarizabilities and hyperpolarizabilities"

The results are quite encouraging. An interesting point is that
comparisons between HF and DFT with overly small basis sets (valence
triple zeta in our case) are dominated by basis set effects instead
of the treatment of exchange and correlation. Thus the quantitative
advantages of DFT only became apparent as the basis sets became more complete.
Of course, convergence rates will depend on the property.

... Mark E. Casida
Return-Path: <casida@CHIMCN.UMontreal.CA>