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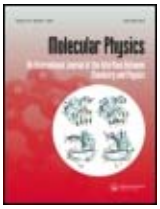

Advances in molecular quantum chemistry contained in the Q-Chem 4 program package

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Yihan Shao[a], Zhengting Gan[a], Evgeny Epifanovsky[abc], Andrew T.B. Gilbert[d], Michael Wormit[e], Joerg Kussmann[f], Adrian W. Lange[g], Andrew Behn[c], Jia Deng[d], Xintian Feng[b], Debashree Ghosh[b], Matthew Goldey[c], Paul R. Horn[c], Leif D. Jacobson[g], Ilya Kaliman[h], Rustam Z. Khaliullin[c], Tomasz Kuś[b], Arie Landau[b], Jie Liu[ig], Emil I. Proynov[a], Young Min Rhee[c], Ryan M. Richard[g], Mary A. Rohrdanz[g], Ryan P. Steele[j], Eric J. Sundstrom[c], H. Lee Woodcock III[ad], Paul M. Zimmerman[ck], Dmitry Zuev[b], Ben Albrecht[l], Ethan Alguire[s], Brian Austin[c], Gregory J. O. Beran[m], Yves A. Bernard[b], Eric Berquist[a], Kai Brandhorst[c], Ksenia B. Bravaya[b], Shawn T. Brown[a], David Casanova[cn], Chung-Min Chang[a], Yunquing Chen[k], Siu Hung Chien[a], Kristina D. Closser[a], Deborah L. Crittenden[d], Michael Diedenhofen[o], Robert A. DiStasio Jr.[c], Hainam Do[p], Anthony D. Dutoi[q], Richard G. Edgar[r], Shervin Fatehi[sj], Laszlo Fusti-Molnar[a], An Ghysels[t], Anna Golubeva-Zadorozhnaya[b], Joseph Gomes[c], Magnus W.D. Hanson-Heine[p], Philipp H.P. Harbach[e], Andreas W. Hauser[c], Edward G. Hohenstein[u], Zachary C. Holden[g], Thomas-C. Jagau[b], Hyunjun Ji[v], Ben Kaduk[w], Kirill Khistyaev[b], Jaehoon Kim[v], Jihan Kim[c], Rollin A. King[x], Phil Klunzinger[y], Dmytro Kosenkov[h], Tim Kowalczyk[w], Caroline M. Krauter[e], Ka Un Lao[g], Adèle Laurent[b], Keith V. Lawler[c], Sergey V. Levchenko[b], Ching Yeh Lin[d], Fenglai Liu[a], Ester Livshits[z], Rohini C. Lochan[c], Arne Luenser[f], Prashant Manohar[b], Samuel F. Manzer[c], Shan-Ping Mao[aa], Narbe Mardirossian[c], Aleksandr V. Marenich[ab], Simon A. Maurer[f], Nicholas J. Mayhall[c], Eric Neuscamman[c], C. Melania Oana[b], Roberto Olivares-Amaya[rac], Darragh P. O'Neill[d], John A. Parkhill[c], Trilisa M. Perrine[k], Roberto Peverati[abc], Alexander Prociuk[k], Dirk R. Rehn[e], Edina Rosta[b], Nicholas J. Russ[a], Shaama M. Sharada[c], Sandeep Sharma[ac], David W. Small[c], Alexander Sodt[ct], Tamar Stein[z], David Stück[c], Yu-Chuan Su[aa], Alex J.W. Thom[c], Takashi Tsuchimochi[w], Vitalii Vanovschi[b], Leslie Vogt[r], Oleg Vydrov[w], Tao Wang[b], Mark A. Watson[acr], Jan Wenzel[e], Alec White[c], Christopher F. Williams[g], Jun Yang[ac], Sina Yeganeh[w], Shane R. Yost[cw], Zhi-Qiang You[aeg], Igor Ying Zhang[af], Xing Zhang[g], Yan Zhao[ab], Bernard R. Brooks[u], Garnet K.L. Chan[ac], Daniel M. Chipman[ag], Christopher J. Cramer[ab], William A. Goddard III[ah], Mark S. Gordon[ai], Warren J. Hehre[y], Andreas Klamt[o], Henry F. Schaefer III[aj], Michael W. Schmidt[ai], C. David Sherrill[u], Donald G. Truhlar[ab], Arieh Warshel[b], Xin Xu[af], Alán Aspuru-Guzik[r], Roi Baer[z], Alexis T. Bell[c], Nicholas A. Besley[p], Jeng-Da Chai[aa], Andreas Dreuw[e], Barry D. Dunietz[ak], Thomas R. Furlani[al], Steven R. Gwaltney[am], Chao-Ping Hsu[ae], Yousung Jung[v], Jing Kong[a], Daniel S. Lambrecht[a], WanZhen Liang[i], Christian Ochsenfeld[f], Vitaly A. Rassolov[an], Lyudmila V. Slipchenko[h], Joseph E. Subotnik[s], Troy Van Voorhis[w], John M. Herbert[g], Anna I. Krylov[b], Peter M.W. Gill[d] & Martin Head-Gordon[c*]

Publishing models and article dates explained

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Abstract

A summary of the technical advances that are incorporated in the fourth major release of the Q-Chem quantum chemistry program is provided, covering approximately the last seven years. These include developments in density functional theory methods and algorithms, nuclear magnetic resonance (NMR) property evaluation, coupled cluster and perturbation theories, methods for electronically excited and open-shell species, tools for treating extended environments, algorithms for walking on potential surfaces, analysis tools, energy and electron transfer modelling, parallel computing capabilities, and graphical user interfaces. In addition, a selection of example case studies that illustrate these capabilities is given. These include extensive benchmarks of the comparative accuracy of modern density functionals for bonded and non-bonded interactions, tests of attenuated second order Møller–Plesset (MP2) methods for intermolecular interactions, a variety of parallel performance benchmarks, and tests of the accuracy of implicit solvation models. Some specific chemical examples include calculations on the strongly correlated Cr_2 dimer, exploring zeolite-catalysed ethane dehydrogenation, energy decomposition analysis of a charged ter-molecular complex arising from glycerol photoionisation, and natural transition orbitals for a Frenkel exciton state in a nine-unit model of a self-assembling nanotube.

Keywords

- quantum chemistry,
- software,
- electronic structure theory,
- density functional theory,
- electron correlation,
- computational modelling,
- Q-Chem

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Author affiliations

- [a] Q-Chem Inc, Pleasanton, CA, USA
- [b] Department of Chemistry, University of Southern California, Los Angeles, CA, USA
- [c] Department of Chemistry, University of California, Berkeley, CA, USA
- [d] Research School of Chemistry, Australian National University, Canberra, Australia
- [e] Interdisciplinary Center for Scientific Computing, Ruprecht-Karls University, Heidelberg, Germany
- [f] Department of Chemistry, University of Munich (LMU), München, Germany
- [g] Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH, USA
- [h] Department of Chemistry, Purdue University, West Lafayette, IN, USA
- [i] Department of Chemistry, Xiamen University, Xiamen, China
- [j] Department of Chemistry, The University of Utah, Salt Lake City, UT, USA
- [k] Department of Chemistry, University of Michigan, Ann Arbor, MI, USA
- [l] Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, USA
- [m] Department of Chemistry, University of California, Riverside, CA, USA
- [n] IKERBASQUE - Basque Foundation for Science & Donostia International Physics Center (DIPC) & Kimika Fakultatea, Euskal Herriko Unibertsitatea (UPV/EHU), Donostia, Spain
- [o] COSMOlogic GmbH & Co. KG, Leverkusen, Germany
- [p] School of Chemistry, The University of Nottingham, Nottingham, United Kingdom
- [q] Department of Chemistry, University of the Pacific, Stockton, CA, USA
- [r] Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, USA
- [s] Department of Chemistry, University of Pennsylvania, Philadelphia, PA, USA
- [t] Computational Biophysics Section, Heart, Lung, and Blood Institute, National Institutes of Health, Bethesda, MD, USA
- [u] School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, USA
- [v] Graduate School of EEWS, KAIST, Daejeon, Republic of Korea
- [w] Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, USA
- [x] Department of Chemistry, Bethel University, St. Paul, MN, USA
- [y] Wavefunction Inc., Irvine, CA, USA
- [z] The Chaim Weizmann Institute of Chemistry, and the Fritz Haber Research Center for Molecular Dynamics, The Hebrew University of Jerusalem, Jerusalem, Israel
- [aa] Department of Physics, National Taiwan University, Taipei, Taiwan
- [ab] Department of Chemistry, University of Minnesota, Minneapolis, MN, USA
- [ac] Department of Chemistry, Princeton University, Princeton, NJ, USA
- [ad] Department of Chemistry, University of South Florida, Tampa, FL, USA
- [ae] Institute of Chemistry, Academia Sinica, Taipei, Taiwan
- [af] Department of Chemistry, Fudan University, Shanghai, China
- [ag] Radiation Laboratory, University of Notre Dame, Notre Dame, IN, USA
- [ah] Materials and Process Simulation Center, California Institute of Technology, Pasadena, CA, USA
- [ai] Department of Chemistry, Iowa State University, Ames, IA, USA
- [aj] Department of Chemistry, University of Georgia, Athens, GA, USA
- [ak] Department of Chemistry and Biochemistry, Kent State University, Kent, OH, USA
- [al] Center for Computational Research, SUNY at Buffalo, Buffalo, NY, USA

- [am] Department of Chemistry, Mississippi State University, Mississippi State, MS, USA
- [an] Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, USA