Curriculum Vitæ

Dmitri G. Fedorov

Present affiliation

Senior Researcher
Materials DX Research Center (MDX)
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Education

Ph.D. in Chemistry, Iowa State University, USA, 1994-1999

Professional experience

2002-now	AIST, Japan
1999-2002	postdoctoral researcher, the University of Tokyo, Japan
1994-1999	research and teaching assistant, Iowa State University, USA

Current research topics

Development and applications of the fragment molecular orbital method.
Study of molecular interactions.
Parallelisation of quantum-mechanical methods for high-performance computing.

Awards

1. JSPS Fellowship, 2000-2001

2. The best technical paper award, Supercomputing 2005, Seattle, USA.
T. Ikegami, T. Ishida, D. G. Fedorov, K. Kitaura, Y. Inadomi, H. Umeda, M. Yokokawa, S. Sekiguchi, Full electron calculation beyond 20,000 atoms: ground electronic state of photosynthetic proteins.

Books

1. D. G. Fedorov, Complete guide to the fragment molecular orbital method in GAMESS, World Scientific, Singapore, 2023.
2. D. G. Fedorov, K. Kitaura, Eds., *The fragment molecular orbital method: practical applications to large molecular systems*. 288 pages. CRC Press, Boca Raton, FL, 2009.

Regular reviewed papers

1. D. G. Fedorov, M. Evans, Y. Song, M. S. Gordon, C. Y. Ng. An experimental and theoretical study of the spin-orbit interaction for CO^+($A\ ^2\Pi_{3/2,1/2}$, ν^+ = 0-41) and O_2^+ ($X\ ^2\Pi_{3/2,1/2g}$, ν^+ = 0-38). J. Chem. Phys. 111 (1999) 6413-6421.
2. D. G. Fedorov, M. S. Gordon. A study of the relative importance of one and two-electron contributions to spin-orbit coupling. J. Chem. Phys. 112 (2000) 5611-5623.
3. J. Moc, D. G. Fedorov, M. S. Gordon. A theoretical study of the reaction of Ti^+ with ethane. J. Chem. Phys. 112 (2000) 10247-10258.
4. D. G. Fedorov, M. S. Gordon. A theoretical study of the reaction paths for cobalt cation + propane, J. Phys. Chem. A 104 (2000) 2253-2260.
5. D. G. Fedorov, T. Nakajima, K. Hirao. Analytic gradient for the relativistic elimination of small components (RESC) approach. Chem. Phys. Lett. 335 (2001) 183-187.
6. S. Koseki, D. G. Fedorov, M. W. Schmidt, M. S. Gordon. Spin-orbit splittings in the third-row transition elements: comparison of effective nuclear charge and full Breit-Pauli calculations. J. Phys. Chem. A 105 (2001) 8262-8268.
7. D. G. Fedorov, M. S. Gordon, Y. Song, C. Y. Ng. Theoretical study of spin-orbit coupling constants for O_2^+ ($A\ ^2\Pi_{3/2,1/2u}$, ν^+ =0-17 and $a\ ^4\Pi_{5/2,3/2,1/2,-1/2u}$, ν^+ = 0-25). J. Chem. Phys. 115 (2001) 7393-7400.
8. D. G. Fedorov, J. P. Finley. Spin-orbit multireference multistate perturbation theory. Phys. Rev. A 64 (2001) 042502.
9. S. Koseki, Y. Ishihara, H. Umeda, D. G. Fedorov, M. S. Gordon. Dissociation potential curves of low-lying states in transition metal hydrides. I. Hydrides of group 4. J. Phys. Chem. A 106 (2002) 785-794.
10. H. A. Witek, D. G. Fedorov, K. Hirao, A. Viel, P.-O. Widmark. Theoretical study of the unusual potential energy curve of the $A\ ^1\Sigma^+$ state of AgH. J. Chem. Phys. 116 (2002) 8396-8406.
11. D. G. Fedorov, M. Klobukowski. Spin-orbit coupling with model core potentials. Chem. Phys. Lett. 360 (2002) 223-228.
12. W. Lie, D. G. Fedorov, K. Hirao. Theoretical Study of the reaction $XY_4 = XY_3+Y$, where X = C, Si, Ge, Sn, Pb and Y = CH_3, C_2H_5. J. Phys. Chem. A 106 (2002) 7057-7061.
13. D. Ajitha, D. G. Fedorov, J. P. Finley, K. Hirao. Photodissociation of alkyl and aryl iodides and effect of fluorination: Analysis of proposed mechanisms and vertical excitations by spin-orbit ab initio study. J. Chem. Phys. 117 (2002) 7068-7076.
14. D. G. Fedorov, T. Nakajima, K. Hirao. An ab initio study of excited states of U and UF. J. Chem. Phys. 118 (2003) 4970-4975.
15. Y. Komeiji, T. Nakano, K. Fukuzawa, Y. Ueno, Y. Inadomi, T. Nemoto, M. Uebayasi, D. G. Fedorov, K. Kitaura. Fragment molecular orbital method: application to molecular dynamics simulation, `ab initio FMO-MD'. Chem. Phys. Lett. 372 (2003) 342-347.
16. D. G. Fedorov, R. M. Olson, K. Kitaura, M. S. Gordon, S. Koseki. A new hierarchical parallelization scheme: generalized distributed data interface (GDDI), and an application to the fragment molecular orbital method (FMO). J. Comput. Chem. 25 (2004) 872-880.

17. D. G. Fedorov, K. Kitaura. The importance of three-body terms in the fragment molecular orbital method. J. Chem. Phys. 120 (2004) 6832-6840.
18. D. G. Fedorov, K. Kitaura. On the accuracy of the 3-body fragment molecular orbital method (FMO) applied to density functional theory. Chem. Phys. Lett. 389 (2004) 129-134.
19. S. Koseki, Y. Ishihara, D. G. Fedorov, H. Umeda, M. W. Schmidt, M. S. Gordon. Dissociation Potential Curves of Low-Lying States in Transition Metal Hydrides. 2. Hydrides of Groups 3 and 5. J. Phys. Chem. A 108 (2004) 4707-4719.
20. D. G. Fedorov, K. Kitaura. Second order Møller-Plesset perturbation theory based upon the fragment molecular orbital method. J. Chem. Phys. 121 (2004) 2483-2490.
21. D. G. Fedorov, K. Kitaura. Multiconfiguration self-consistent-field theory based upon the fragment molecular orbital method. J. Chem. Phys. 122 (2005) 054108.
22. D. G. Fedorov, T. Ishida, K. Kitaura. Multilayer formulation of the fragment molecular orbital method (FMO). J. Phys. Chem. A. 109 (2005) 2638-2646.
23. D. G. Fedorov, K. Kitaura. Coupled-cluster theory based upon the fragment molecular-orbital method. J. Chem. Phys. 123 (2005) 134103.
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25. T. Nemoto, D. G. Fedorov, M. Uebayasi, K. Kanazawa, K. Kitaura, Y. Komeiji. Ab initio fragment molecular orbital (FMO) method applied to analysis of the ligand-protein interaction in a pheromone-binding protein. Comput. Biol. Chem. 29 (2005) 434-439.
26. T. Ishida, D. G. Fedorov, K. Kitaura. All electron quantum chemical calculation of the entire enzyme system confirms a collective catalytic device in the chorismate mutase reaction. J. Phys. Chem. B 110 (2006) 1457-1463.
27. D. G. Fedorov, K. Kitaura, H. Li, J. H. Jensen, M. S. Gordon. The polarizable continuum model (PCM) interfaced with the fragment molecular orbital method (FMO). J. Comput. Chem. 27 (2006) 976-985.
28. P. V. Avramov, P. B. Sorokin, A. S. Fedorov, D. G. Fedorov, Y. Maeda. Band-gap unification of partially Si-substituted single-wall carbon nanotubes. Phys. Rev. B 74 (2006) 245417.
29. D. G. Fedorov, K. Kitaura. The three-body fragment molecular orbital method for accurate calculations of large systems. Chem. Phys. Lett. 433 (2006) 182-187.
30. D. G. Fedorov, K. Kitaura. Pair interaction energy decomposition analysis. J. Comput. Chem. 28 (2007) 222-237.
31. D. G. Fedorov, T. Ishida, M. Uebayasi, K. Kitaura. The fragment molecular orbital method for geometry optimizations of polypeptides and proteins. J. Phys. Chem. A 111 (2007) 2722-2732.
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33. I. Nakanishi, D. G. Fedorov, K. Kitaura. Molecular recognition mechanism of FK506 binding protein: An all-electron fragment molecular orbital study. Proteins: Struct., Funct., Bioinf. 68 (2007) 145-158.

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51. T. Zeng, D. G. Fedorov, M. Klobukowski, Model core potentials for studies of scalar-relativistic effects and spin-orbit coupling at Douglas-Kroll level. I. Theory and applications to Pb and Bi. J. Chem. Phys. 131, 124109 (2009).
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66. D. G. Fedorov, Y. Alexeev, K. Kitaura. Geometry optimization of the active site of a large system with the fragment molecular orbital method. J. Phys. Chem. Lett. 2 (2011) 282-288.
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