Ivan S Ufimtsev

List of Publications by Year
in descending order

25	3,533	471509 17	642732 23
papers	citations	h-index	g-index

25	25	25	2686
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>TeraChem</scp>: A graphical processing unit<scp>â€accelerated</scp> electronic structure package for <scp>largeâ€scale</scp> ab initio molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1494.	14.6	143
2	Cover Image, Volume 11, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1523.	14.6	5
3	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. Journal of Chemical Physics, 2020, 152, 224110.	3.0	87
4	Structural insights into the aPKC regulatory switch mechanism of the human cell polarity protein lethal giant larvae 2. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10804-10812.	7.1	13
5	Unsupervised determination of protein crystal structures. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10813-10818.	7.1	4
6	Solving the structure of Lgl2, a difficult blind test of unsupervised structure determination. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10819-10823.	7.1	5
7	Analytic first derivatives of floating occupation molecular orbital-complete active space configuration interaction on graphical processing units. Journal of Chemical Physics, 2015, 143, 014111.	3.0	44
8	An atomic orbital-based formulation of the complete active space self-consistent field method on graphical processing units. Journal of Chemical Physics, 2015, 142, 224103.	3.0	98
9	Generating Efficient Quantum Chemistry Codes for Novel Architectures. Journal of Chemical Theory and Computation, 2013, 9, 213-221.	5.3	316
10	Ab Initio Quantum Chemistry for Protein Structures. Journal of Physical Chemistry B, 2012, 116, 12501-12509.	2.6	99
11	Porting Optimized GPU Kernels to a Multi-core CPU: Computational Quantum Chemistry Application Example. , 2011, , .		4
12	Dynamic Precision for Electron Repulsion Integral Evaluation on Graphical Processing Units (GPUs). Journal of Chemical Theory and Computation, 2011, 7, 949-954.	5.3	138
13	Charge Transfer and Polarization in Solvated Proteins from Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2011, 2, 1789-1793.	4.6	113
14	Excited-State Electronic Structure with Configuration Interaction Singles and Tammâ€“Dancoff Time-Dependent Density Functional Theory on Graphical Processing Units. Journal of Chemical Theory and Computation, 2011, 7, 1814-1823.	5.3	180
15	GPU-accelerated molecular modeling coming of age. Journal of Molecular Graphics and Modelling, 2010, 29, 116-125.	2.4	336
16	Direct self-consistent field computations on GPU clusters. , 2010, , .		6
17	Implementation of Scientific Computing Applications on the Cell Broadband Engine. Scientific Programming, 2009, 17, 135-151.	0.7	7
18	Observation of a Zundel-like transition state during proton transfer in aqueous hydroxide solutions. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15154-15159.	7.1	111

#	Article	IF	Citations
19	Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field Implementation. Journal of Chemical Theory and Computation, 2009, 5, 1004-1015.	5.3	354
20	Quantum Chemistry on Graphical Processing Units. 3. Analytical Energy Gradients, Geometry Optimization, and First Principles Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 2619-2628.	5.3	734
21	Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field (SCF) Implementation. Journal of Chemical Theory and Computation, 2009, 5, 3138-3138.	5.3	18
22	A multistate empirical valence bond model for solvation and transport simulations of OHâ˜ in aqueous solutions. Physical Chemistry Chemical Physics, 2009, 11, 9420.	2.8	45
23	Quantum Chemistry on Graphical Processing Units. 1. Strategies for Two-Electron Integral Evaluation. Journal of Chemical Theory and Computation, 2008, 4, 222-231.	5.3	458
24	Graphical Processing Units for Quantum Chemistry. Computing in Science and Engineering, 2008, 10, 26-34.	1.2	169
25	A charged ring model for classical OHâ˜(aq) simulations. Chemical Physics Letters, 2007, 442, 128-133.	2.6	46