Alistair P Rendell

List of Publications by Year
in descending order

109	5,128	136740	91712
papers	citations	32 h-index	69 g-index

112	112	112	4100
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
2	The restricted active space self-consistent-field method, implemented with a split graph unitary group approach. The Journal of Physical Chemistry, 1990, 94, 5477-5482.	2.9	621
3	Modeling nonlinear ultrasound propagation in heterogeneous media with power law absorption using a k-space pseudospectral method. Journal of the Acoustical Society of America, 2012, 131, 4324-4336.	0.5	372
4	Comparison of the quadratic configuration interaction and coupled-cluster approaches to electron correlation including the effect of triple excitations. The Journal of Physical Chemistry, 1990, 94, 5463-5468.	2.9	311
5	Coupledâ€cluster theory employing approximate integrals: An approach to avoid the input/output and storage bottlenecks. Journal of Chemical Physics, 1994, 101, 400-408.	1.2	183
6	Analytic gradients for coupledâ€cluster energies that include noniterative connected triple excitations: Application to cisâ€•and transâ€HONO. Journal of Chemical Physics, 1991, 94, 6229-6236.	1.2	172
7	The potassium channel: Structure, selectivity and diffusion. Journal of Chemical Physics, 2000, 112, 8191-8204.	1.2	134
8	The structure and energetics of the HCN â†' HNC transition state. Chemical Physics Letters, 1991, 177, 491-497.	1.2	112
9	Openâ€shell restricted Hartreeâ€“Fock perturbation theory: Some considerations and comparisons. Journal of Chemical Physics, 1994, 100, 7400-7409.	1.2	92
10	The validity of electrostatic predictions of the shapes of van der Waals dimers. Chemical Physics Letters, 1985, 117, 400-408.	1.2	89
11	Binding energies and bond distances of Ni(CO)x,x=1â€“4: An application of coupledâ€cluster theory. Journal of Chemical Physics, 1991, 95, 5898-5905.	1.2	84
12	Vibrational frequencies for Be3 and Be4. Journal of Chemical Physics, 1990, 92, 7050-7056.	1.2	82
13	A parallel vectorized implementation of triple excitations in CCSD(T): application to the binding energies of the AlH3, AlH2F, AlHF2 and AlF3 dimers. Chemical Physics Letters, 1991, 178, 462-470.	1.2	78
14	A parallel second-order MÃ¸ller-Plesset gradient. Molecular Physics, 1997, 91, 431-438.	0.8	78
15	Electrostatics for Exploring Hydration Patterns of Molecules. 3. Uracil. Journal of Physical Chemistry A, 2000, 104, 8976-8982.	1.1	74
16	An efficient formulation and implementation of the analytic energy gradient method to the single and double excitation coupledâ€cluster wave function: Application to Cl2O2. Journal of Chemical Physics, 1991, 94, 6219-6228.	1.2	68
17	A direct coupled cluster algorithm for massively parallel computers. Chemical Physics Letters, 1997, 265, 1-11.	1.2	68
18	Theoretical investigations of the structures and binding energies of Ben and Mgn(n=3â€“5) clusters. Journal of Chemical Physics, 1990, 92, 489-495.	1.2	63

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19	Quantum chemistry on parallel computer architectures: coupled-cluster theory applied to the bending potential of fulminic acid. Chemical Physics Letters, 1992, 194, 84-94.	1.2	63
20	Use of SIMD Vector Operations to Accelerate Application Code Performance on Low-Powered ARM and Intel Platforms. , 2013, , .		60
21	Structures, Relative Stabilities, and Spectra of Isomers of HClO2. The Journal of Physical Chemistry, 1994, 98, 5644-5649.	2.9	54
22	Triple and quadruple excitation contributions to the binding in Be clusters: Calibration calculations on Be3. Journal of Chemical Physics, 1990, 93, 8875-8880.	1.2	50
23	Full-wave nonlinear ultrasound simulation on distributed clusters with applications in high-intensity focused ultrasound. International Journal of High Performance Computing Applications, 2016, 30, 137-155.	2.4	50
24	Distributed data parallel coupled-cluster algorithm: Application to the 2-hydroxypyridine/2-pyridone tautomerism. Journal of Computational Chemistry, 1993, 14, 1429-1439.	1.5	46
25	Liquid water. , 2009, , .		44
26	Validity of current force fields for simulations on boron nitride nanotubes. Micro and Nano Letters, 2010, 5, 150.	0.6	44
27	Vibrations in small Mg clusters. Journal of Chemical Physics, 1990, 93, 6636-6641.	1.2	43
28	The analytic configuration interaction gradient method: The calculation of one electron properties. Journal of Chemical Physics, 1987, 87, 5976-5986.	1.2	39
29	Parallel direct four-index transformations. Theoretica Chimica Acta, 1996, 93, 317-331.	0.9	37
30	An ab initio quantum chemical study of vertically excited singlet states of pyrimidine. Chemical Physics, 1992, 162, 359-367.	0.9	36
31	Ab initio characterization of peroxyhypochlorous acid: implications for atmospheric chemistry. The Journal of Physical Chemistry, 1993, 97, 6999-7002.	2.9	35
32	Comparison of enzyme polarization of ligands and charge-transfer effects for dihydrofolate reductase using point-charge embeddedab initio quantum mechanical and linear-scaling semiempirical quantum mechanical methods. Journal of Computational Chemistry, 2000, 21, 788-811.	1.5	35
33	Comparison of linear-scaling semiempirical methods and combined quantum mechanical/molecular mechanical methods applied to enzyme reactions. Chemical Physics Letters, 2000, 320, 169-176.	1.2	35
34	Exploring Thread and Memory Placement on NUMA Architectures: Solaris and Linux, UltraSPARC/FirePlane and Opteron/HyperTransport. Lecture Notes in Computer Science, 2006, , 338-352.	1.0	34
35	Enabling the Efficient Use of SMP Clusters. , 2003, , .		33
36	Automatically generated Coulomb fitting basis sets: Design and accuracy for systems containing H to Kr. Journal of Chemical Physics, 2007, 127, 074102.	1.2	33

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37	Evaluation of the contribution from triply excited intermediates to the fourth-order perturbation theory energy on Intel distributed memory supercomputers. Theoretica Chimica Acta, 1993, 84, 271-287.	0.9	32
38	Abinitioquantum chemical study of the molecular and spectroscopic (infrared and Raman) properties of sulfur dioxide: Comparison with ozone. Journal of Chemical Physics, 1988, 89, 5721-5730.	1.2	31
39	An ab initio quantum chemical study of the hydrogenâ€•and â€˜â€˜antiâ€™â€™â€hydrogenâ€bonded HF/ClF and HF/Cl2 dimers. Journal of Chemical Physics, 1987, 87, 535-544.	1.2	30
40	Investigation of a diagnostic for perturbation theory. Comparison to the T1 diagnostic of coupled-cluster theory. Chemical Physics Letters, 1995, 243, 402-408.	1.2	28
41	Silicon Carbide Nanotube as a Chloride-Selective Channel. Journal of Physical Chemistry C, 2012, 116, 4465-4470.	1.5	28
42	Novel Computer Architectures and Quantum Chemistry. Journal of Physical Chemistry A, 2020, 124, 4557-4582.	1.1	27
43	Computational Methods for the Study of Enzymic Reaction Mechanisms. 1. Application to the Hydride Transfer Step in the Catalysis of Dihydrofolate Reductase. Journal of Physical Chemistry B, 2002, 106, 9934-9944.	1.2	26
44	Comparison of linear-scaling semiempirical methods and combined quantum mechanical/molecular mechanical methods for enzymic reactions. II. An energy decomposition analysis. Journal of Computational Chemistry, 2002, 23, 1314-1322.	1.5	26
45	OpenMP on the Low-Power TI Keystone II ARM/DSP System-on-Chip. Lecture Notes in Computer Science, 2013, , 114-127.	1.0	26
46	Implementation and Optimization of the OpenMP Accelerator Model for the TI Keystone II Architecture. Lecture Notes in Computer Science, 2014, , 202-214.	1.0	26
47	The Potassium Ion Channel:Â Comparison of Linear Scaling Semiempirical and Molecular Mechanics Representations of the Electrostatic Potential. Journal of Physical Chemistry B, 2001, 105, 12674-12679.	1.2	25
48	Programming the Adapteva Epiphany 64-Core Network-on-Chip Coprocessor. , 2014, , .		25
49	High-Performance, Graphics Processing Unit-Accelerated Fock Build Algorithm. Journal of Chemical Theory and Computation, 2020, 16, 7232-7238.	2.3	25
50	Theoretical study of the radiative lifetime of the Aâ€‰1âˆ‘u state of C2. Journal of Chemical Physics, 1990, 92, 3000-3004.	1.2	24
51	Enzyme polarization of substrates of dihydrofolate reductase by different theoretical methods. , 1999, 37, 157-165.		23
52	Modelling the bacterial photosynthetic reaction center. VI. Use of density-functional theory to determine the nature of the vibronic coupling between the four lowest-energy electronic states of the special-pair radical cation. Journal of Chemical Physics, 2003, 119, 3249-3261.	1.2	23
53	Faster Self-Consistent Field (SCF) Calculations on GPU Clusters. Journal of Chemical Theory and Computation, 2021, 17, 7486-7503.	2.3	23
54	Electronic Effects in Biomolecular Simulations:Â Investigation of the KcsA Potassium Ion Channel. Journal of Physical Chemistry B, 2004, 108, 13866-13873.	1.2	22

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55	First-Principles Study of Water Confined in Single-Walled Silicon Carbide Nanotubes. Journal of Physical Chemistry C, 2011, 115, 17255-17264.	1.5	22
56	Quantum Chemical Calculations Using Accelerators: Migrating Matrix Operations to the NVIDIA Kepler GPU and the Intel Xeon Phi. Journal of Chemical Theory and Computation, 2014, 10, 908-912.	2.3	22
57	Electrostatic investigation of metal cation binding to DNA bases and base pairs. Chemical Communications, 1998, , 573-574.	2.2	21
58	X10 as a Parallel Language for Scientific Computation: Practice and Experience. , 2011, , .		21
59	Generating optimal CUDA sparse matrix-vector product implementations for evolving GPU hardware. Concurrency Computation Practice and Experience, 2012, 24, 3-13.	1.4	20
60	The role of electrostatics in molecular interactions: prediction of shapes and electronic properties of weakly bound complexes. International Reviews in Physical Chemistry, 1986, 5, 139-146.	0.9	18
61	Electron transfer via dithiaspiroalkane linkages. Nature of long-range through-bond electronic coupling in disulfoxide radical cations and bis(metal) complexes and implications for the characterization of the sulfoxide bond. Journal of the American Chemical Society, 1988, 110, 8343-8354.	6.6	18
62	Ab initiopotential-energy curves for the molecular ions NeH+and ArH+. Molecular Physics, 1992, 77, 279-290.	0.8	18
63	The structures, binding energies and vibrational frequencies of Ca3 and Ca4 ? An application of the CCSD(T) method. Theoretica Chimica Acta, 1992, 83, 165-175.	0.9	18
64	A theoretical determination of the radiative lifetimes of the A 2Î£+ and B 2Î” states of CF. Chemical Physics Letters, 1989, 163, 354-358.	1.2	17
65	Comparison of semiempirical and ab initio QM decomposition analyses for the interaction energy between molecules. Chemical Physics Letters, 2002, 352, 245-251.	1.2	17
66	Energy-Efficient Computational Chemistry: Comparison of x86 and ARM Systems. Journal of Chemical Theory and Computation, 2015, 11, 5055-5061.	2.3	17
67	Theoretical study of the radiative lifetime of the Aâ€‰1âˆ‘u state of C2. Journal of Chemical Physics, 1990, 92, 6599-6603.	1.2	16
68	Fault-Tolerant Grid-Based Solvers: Combining Concepts from Sparse Grids and MapReduce. Procedia Computer Science, 2013, 18, 130-139.	1.2	15
69	First Principles Study of Gallium Atom Adsorption on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2006, 110, 9608-9618.	1.2	14
70	The spectroscopy of MnH. Journal of Molecular Spectroscopy, 1989, 138, 108-122.	0.4	13
71	Diagonalization-free SCF. Chemical Physics Letters, 1994, 229, 204-210.	1.2	13
72	On the orbital contribution to analytical derivatives of perturbation theory energies. Molecular Physics, 1995, 85, 561-571.	0.8	13

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73	Dynamic Algorithm Selection Using Reinforcement Learning. , 2006, , .		13
74	Profiling Directed NUMA Optimization on Linux Systems: A Case Study of the Gaussian Computational Chemistry Code. , 2011, , .		12
75	Scaling the Hartree-Fock Matrix Build on Summit. , 2020, , .		10
76	High-Performance Pseudo-Random Number Generation on Graphics Processing Units. Lecture Notes in Computer Science, 2012, , 609-618.	1.0	9
77	From Sparse Matrix to Optimal GPU CUDA Sparse Matrix Vector Product Implementation. , 2010, , .		8
78	Computational chemistry on Fujitsu vectorâ€“parallel processors: Development and performance of applications software. Parallel Computing, 2000, 26, 887-911.	1.3	7
79	Modelling the Runtime of the Gaussian Computational Chemistry Application and Assessing the Impacts of Microarchitectural Variations. Procedia Computer Science, 2011, 4, 281-291.	1.2	7
80	Programming the Adapteva Epiphany 64-core network-on-chip coprocessor. International Journal of High Performance Computing Applications, 2017, 31, 285-302.	2.4	7
81	The design of MPI based distributed shared memory systems to support OpenMP on clusters. , 2007, , .		6
82	Placing Rigorous Bounds on Numerical Errors in Hartreeâ€“Fock Energy Computations. Journal of Chemical Theory and Computation, 2011, 7, 1631-1639.	2.3	6
83	Resolutions of the Coulomb Operator: VII.ÂEvaluationÂofÂLong-RangeÂCoulombÂandÂExchangeÂMatrices. Journal of Chemical Theory and Computation, 2013, 9, 863-867.	2.3	6
84	OpenMP and NUMA Architectures I: Investigating Memory Placement on the SGI Origin 3000. Lecture Notes in Computer Science, 2003, , 648-656.	1.0	5
85	Effective Use of Dynamic Page Migration on NUMA Platforms: The Gaussian Chemistry Code on the SunFire X4600M2 System. , 2009, , .		5
86	Runtime sparse matrix format selection. Procedia Computer Science, 2010, 1, 135-144.	1.2	5
87	Implementation of 3D FFTs Across Multiple GPUs in Shared Memory Environments. , 2012, , .		5
88	Interval Arithmetic and Computational Science: Rounding and Truncation Errors in N-Body Methods. , 2007, , .		4
89	Ga Cleaning of Al2O3 Substrate:â€‰ Low Coverage Adsorption of Ga on a Hydrogen-Contaminated Î±-Al2O3(0001) Surface. Journal of Physical Chemistry C, 2007, 111, 3384-3392.	1.5	4
90	Reinforcement learning for automated performance tuning: Initial evaluation for sparse matrix format selection. , 2008, , .		4

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91	Performance models for Cluster-enabled OpenMP implementations. , 2008, , .		4
92	Computational chemistry on Fujitsu vectorâ€“parallel processors: Hardware and programming environment. Parallel Computing, 2000, 26, 869-886.	1.3	3
93	Modelling the Performance of the Gaussian Chemistry Code on x86 Architectures. , 2008, , 49-58.		3
94	Use of Cluster OpenMP with the Gaussian Quantum Chemistry Code: A Preliminary Performance Analysis. Lecture Notes in Computer Science, 2009, , 53-62.	1.0	3
95	Faster gradients for semiempirical methods. Journal of Computational Chemistry, 1999, 20, 629-635.	1.5	2
96	Region-Based Prefetch Techniques for Software Distributed Shared Memory Systems. , 2010, , .		2
97	Deterministic global optimization in ab-initio quantum chemistry. Journal of Global Optimization, 2013, 56, 537-558.	1.1	2
98	PGASâ€FMM: Implementing a distributed fast multipole method using the X10 programming language. Concurrency Computation Practice and Experience, 2014, 26, 712-727.	1.4	2
99	Development and Application of a Hybrid Programming Environment on an ARM/DSP System for High Performance Computing. , 2018, , .		2
100	Non-threaded and Threaded Approaches to MultiRail Communication with uDAPL. , 2009, , .		1
101	Efficient update of ghost regions using active messages. , 2012, , .		1
102	First principles study of galliumâ€cleaning for hydrogenâ€contaminated Î±â€Al₂O₃(0001) surfaces. Journal of Computational Chemistry, 2013, 34, 1101-1111.	1.5	1
103	Embedded Accelerators for Scientific High-Performance Computing: An Energy Study of OpenCL Gaussian Elimination Workloads. , 2017, , .		1
104	Introducing Design Patterns, Graphical User Interfaces and Threads Within the Context of a High Performance Computing Application. Lecture Notes in Computer Science, 2005, , 18-26.	1.0	1
105	The SCore Cluster Enabled OpenMP Environment: Performance Prospects for Computational Science. Lecture Notes in Computer Science, 2005, , 1067-1075.	1.0	0
106	Including Rigorous Numerical Bounds in Quantum Chemistry Calculations: Gaussian Integral Evaluation. , 2008, , .		0
107	Resolutions of the Coulomb operator: VIII. Parallel implementation using the modern programming language X10. Journal of Computational Chemistry, 2014, 35, 2056-2069.	1.5	0
108	A Project Based Approach to Teaching Parallel Systems. Lecture Notes in Computer Science, 2006, , 155-160.	1.0	0

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109	On the Use of Incomplete LU Decomposition as a Preconditioning Technique for Density Fitting in Electronic Structure Computations. , 2007, , 265-280.		0