John A Montgomery Jr

List of Publications by Year
in descending order

33 papers	21,085 citations	586496 16 h-index	466096 32 g-index
33 all docs	33 docs citations	33 times ranked	17475 citing authors

#	Article	IF	Citations
1	Benchmark comparison of dual-basis double-hybrid density functional theory and a neural-network-optimized method for intermolecular interactions. Journal of Molecular Spectroscopy, 2021, 376, 111406.	0.4	5
2	Photoassociation of ultracold long-range polyatomic molecules. Physical Review Research, 2021, 3, .	1.3	8
3	Reaction blockading in a reaction between an excited atom and a charged molecule at low collision energy. Nature Chemistry, 2019, 11, 615-621.	6.6	41
4	Microwave spectroscopy and curious molecular dynamics of ethyl trifluoroacetate. Journal of Molecular Spectroscopy, 2017, 335, 13-16.	0.4	2
5	Synthesis of mixed hypermetallic oxide BaOCa ⁺ from laser-cooled reagents in an atom-ion hybrid trap. Science, 2017, 357, 1370-1375.	6.0	58
6	Predictive coupled-cluster isomer orderings for some SinCm (m, n â‰¤ 12) clusters: A pragmatic comparison between DFT and complete basis limit coupled-cluster benchmarks. Journal of Chemical Physics, 2016, 145, 024312.	1.2	14
7	Second moments and rotational spectroscopy. Journal of Molecular Spectroscopy, 2016, 325, 42-49.	0.4	48
8	Production ofNaCa+molecular ions in the ground state from cold atom-ion mixtures by photoassociation via an intermediate state. Physical Review A, 2016, 94, .	1.0	20
9	At What Chain Length Do Unbranched Alkanes Prefer Folded Conformations?. Journal of Physical Chemistry A, 2014, 118, 1706-1712.	1.1	64
10	Associative detachment of rubidium hydroxide. Physical Review A, 2013, 88, .	1.0	7
11	Structure, energetics, and reactions of alkali tetramers. Journal of Chemical Physics, 2012, 136, 014306.	1.2	16
12	Controllable Binding of Polar Molecules and Metastability of One-Dimensional Gases with Attractive Dipole Forces. Physical Review Letters, 2012, 109, 083003.	2.9	14
13	A QM/MM approach for the study of monolayer-protected gold clusters. Journal of Materials Science, 2012, 47, 7686-7692.	1.7	12
14	Ab initio potential curves for the <mml:math altimg="si62.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.. Chem	1.2	15
15	Long-range forces between polar alkali-metal diatoms aligned by external electric fields. Physical Review A, 2012, 86, .	1.0	16
16	Long-range three-body atomâ€“diatom potential for doublet Li3. Chemical Physics Letters, 2012, 529, 23-26.	1.2	2
17	Long-range interactions between like homonuclear alkali metal diatoms. Journal of Chemical Physics, 2011, 135, 244307.	1.2	22
18	Microwave spectroscopy and conformations of 2-methylbutane and 2,3-dimethylbutane. Journal of Molecular Structure, 2010, 978, 11-13.	1.8	5

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19	Ab initio potential curves for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si45.gif" display="inline" overflow="scroll"><mml:mrow><mml:mtext>X</mml:mtext><mml:msup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup><mml:msubsup><mml:mrow><mml:mi	1.2	18
20	Structure and thermochemistry of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">K</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>Rb, KRb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>, and<mml:m	1.0	44
21	Helical C₂ Structure of Perfluoropentane and the C_{2v} Structure of Perfluoropropane. Journal of Physical Chemistry A, 2010, 114, 1118-1122.	1.1	32
22	Rotational Spectrum, Tunneling Motions, and Potential Barriers of Benzyl Alcohol. Journal of Physical Chemistry A, 2010, 114, 6913-6916.	1.1	34
23	Long range intermolecular interactions between the alkali diatomics Na2, K2, and NaK. Journal of Chemical Physics, 2010, 132, 244305.	1.2	12
24	Potential energy surface of the 1²Aâ€² Li₂ + Li doublet ground state. International Journal of Quantum Chemistry, 2009, 109, 3112-3119.	1.0	9
25	Electronic structure of the Li2 [X ¹Î£] Li [²p] excited ²Aâ€³ surface. International Journal of Quantum Chemistry, 2009, 109, 3626-3631.	1.0	2
26	Unrestricted Coupled Cluster and Brueckner Doubles Variations of W1 Theory. Journal of Chemical Theory and Computation, 2009, 5, 2687-2693.	2.3	232
27	Combining Quantum Mechanics Methods with Molecular Mechanics Methods in ONIOM. Journal of Chemical Theory and Computation, 2006, 2, 815-826.	2.3	855
28	A restricted-open-shell complete-basis-set model chemistry. Journal of Chemical Physics, 2006, 125, 094106.	1.2	208
29	On the optimization of Gaussian basis sets. Journal of Chemical Physics, 2003, 118, 1101-1109.	1.2	61
30	An overlap criterion for selection of core orbitals. Theoretical Chemistry Accounts, 2002, 107, 180-186.	0.5	16
31	Transition states for chemical reactions I. Geometry and classical barrier height. Journal of Chemical Physics, 1998, 108, 5704-5713.	1.2	173
32	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	1.5	19,020
33	Model of Charge Transfer Collisions between C₆₀ and Slow Ions. Journal of Chemical Physics, 0, , .	1.2	0