RamÃ³n HernÃ¡ndez-Lamoneda

List of Publications by Year
in descending order

71 papers	1,159 citations	361045 20 h-index	454577 30 g-index
74 all docs	74 docs citations	74 times ranked	749 citing authors

#	Article	IF	Citations
1	On the Unusual Properties of Halogen Bonds: A Detailed ab Initio Study of X₂â^'(H₂O)_{1â^'5} clusters (X = Cl and Br). Journal of Physical Chemistry A, 2009, 113, 5496-5505.	1.1	62
2	Protonated Isobutane. A Theoretical ab Initio Study of the Isobutonium Cations. Journal of the American Chemical Society, 1997, 119, 5193-5199.	6.6	56
3	Potential Energy Surface of the C3H9+Cations. Protonated Propane. Journal of the American Chemical Society, 1998, 120, 3213-3219.	6.6	49
4	Interaction of NO(Aâ€‰Î£2+) with rare gas atoms: Potential energy surfaces and spectroscopy. Journal of Chemical Physics, 2008, 129, 244303.	1.2	47
5	The intermolecular potentials of the O2â€“O2 dimer: a detailed ab initio study of the energy splittings for the three lowest multiplet states. Physical Chemistry Chemical Physics, 2008, 10, 5374.	1.3	46
6	Reactivity and electronic states of O4 along minimum energy paths. Journal of Chemical Physics, 2000, 113, 4139-4145.	1.2	45
7	Does ozone have a barrier to dissociation and recombination?. Chemical Physics Letters, 2002, 355, 478-482.	1.2	44
8	Longâ€range interaction for dimers of atmospheric interest: dispersion, induction and electrostatic contributions for O₂ï£¿O₂, N₂ï£¿N₂and O₂ï£¿N₂. Journal of Computational Chemistry, 2011, 32, 279-290.	1.5	44
9	Intermolecular Potential of the O2â^'O2Dimer. An ab Initio Study and Comparison with Experimentâ€. Journal of Physical Chemistry A, 2005, 109, 11587-11595.	1.1	39
10	Global ab initio potential energy surfaces for the O2(Î£3gâ^')+O2(Î£3gâ^') interaction. Journal of Chemical Physics, 2010, 133, 124311.	1.2	39
11	3,5-Dimethyl and 3,5-Di-tert-butylpyrazolato Complexes with Alkali Metals:â€‰ Monomeric, Dimeric, Cluster, and 1D Chain Structures. Inorganic Chemistry, 2006, 45, 286-294.	1.9	30
12	Jump in depletion rates of highly excited O2: reaction or enhanced vibrational relaxation?. Chemical Physics Letters, 1998, 289, 150-155.	1.2	29
13	Accurate ab initio intermolecular potential energy surface for the quintet state of the O2(Î£gâ^'3)â€“O2(Î£gâ^'3) dimer. Journal of Chemical Physics, 2008, 128, 214304.	1.2	29
14	The intermolecular potential of NO(A2Î£)â€“Ne: An ab initio study. Chemical Physics Letters, 2006, 421, 389-394.	1.2	26
15	Multireference Quantum Monte Carlo Study of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>Molecule. Physical Review Letters, 2007, 99, 153001.	2.9	26
16	Molecular oxygen tetramer (O2)4: Intermolecular interactions and implications for theÎµsolid phase. Physical Review B, 2011, 84, .	1.1	25
17	Graphene multi-protonation: A cooperative mechanism for proton permeation. Carbon, 2019, 144, 724-730.	5.4	25
18	Two-Dimensional H₂Oâ^'Cl₂ and H₂Oâ^'Br₂ Potential Surfaces:â€‰ An Ab Initio Study of Ground and Valence Excited Electronic States. Journal of Physical Chemistry A, 2008, 112, 89-96.	1.1	22

#	Article	IF	Citations
19	Title is missing!. Topics in Catalysis, 1998, 6, 163-168.	1.3	20
20	The <mml:math altimg="si8.gif" display="inline" 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.com/x	1.2	20
21	Quantum-Mechanical Study of the Collision Dynamics of O₂(³Î£_g^{â¯}) + O₂(³Î£_g^{â¯}) on a New ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2009, 113, 14952-14960.	1.1	20
22	Halogen Bonds in Clathrate Cages: A Real Space Perspective. ChemPhysChem, 2018, 19, 2512-2517.	1.0	20
23	Spin-orbit coupling in O2(Ï...)+O2 collisions: I. Electronic structure calculations on dimer states involving the XÎ£gâ¯3, aÎ”g1, and bÎ£g+1 states of O2. Journal of Chemical Physics, 2005, 123, 074311.	1.2	17
24	Communication: Evidence of halogen bonds in clathrate cages. Journal of Chemical Physics, 2016, 145, 161104.	1.2	17
25	Energy exchange rate coefficients from vibrational inelastic O2(Î£gâ¯3) + O2(Î£gâ¯3) collisions on a new spin-averaged potential energy surface. Journal of Chemical Physics, 2021, 154, 064304.	1.2	17
26	Theoretical evidence for the reaction O2(Ï...) + O2(Ï... = 0) â† O3(X1A1) + O(3P). Chemical Physics Letters, 1997, 276, 152-156.	1.2	16
27	Spinâ€“orbit coupling in highly vibrationally excited O2(v) and O2(v=0)â€“O2(v). Chemical Physics Letters, 2000, 321, 191-196.	1.2	15
28	Systematic ab initio calculations on the energetics and stability of covalent O4. Journal of Chemical Physics, 2004, 120, 10084-10088.	1.2	15
29	Understanding the Îµ and Î¶ High-Pressure Solid Phases of Oxygen. Systematic Periodic Density Functional Theory Studies Using Localized Atomic Basis. Journal of Chemical Theory and Computation, 2015, 11, 1195-1205.	2.3	15
30	A new singlet ab initio potential energy surface for studying vibrational relaxation in O2(v)+O2 collisions. Chemical Physics Letters, 2003, 368, 709-716.	1.2	13
31	Performance of local correlation methods for halogen bonding: The case of Br2â€“(H2O)n,n = 4,5 clusters and Br2@51262 clathrate cage. Journal of Chemical Physics, 2015, 143, 094305.	1.2	13
32	Motion of Br₂ Molecules in Clathrate Cages. A Computational Study of the Dynamic Effects on Its Spectroscopic Behavior. Journal of Physical Chemistry A, 2015, 119, 452-459.	1.1	12
33	Spinâ€“orbit coupling in O2(v)+O2 collisions: A new energy transfer mechanism. Journal of Chemical Physics, 2004, 120, 10355-10358.	1.2	11
34	Electronic excited-state mixing in NeCl2. Journal of Chemical Physics, 2005, 123, 161102.	1.2	11
35	Spin-orbit coupling in O2(v)+O2 collisions. II. Quantum scattering calculations on dimer states involving the XÎ£gâ¯3, aÎ”g1, and bÎ£g+1 states of O2. Journal of Chemical Physics, 2007, 126, 194309.	1.2	11
36	Large Shift and Small Broadening of Br₂ Valence Band upon Dimer Formation with H₂O: An Ab Initio Study. Journal of Physical Chemistry A, 2011, 115, 5983-5991.	1.1	11

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37	Ab initiorovibrational structure of the lowest singlet state of O2-O2. Journal of Chemical Physics, 2012, 137, 114304.	1.2	11
38	Chemical Interactions and Spin Structure in (O₂)₄: Implications for the Îµ-O₂ Phase. Journal of Chemical Theory and Computation, 2013, 9, 2179-2188.	2.3	11
39	NeCl₂ and ArCl₂: Transition from Direct Vibrational Predissociation to Intramolecular Vibrational Relaxation and Electronic Nonadiabatic Effects. Journal of Physical Chemistry A, 2010, 114, 3050-3059.	1.1	10
40	Properties of the molecular oxygen trimer from pairwise additive interactions. Chemical Physics, 2012, 399, 80-85.	0.9	10
41	Permeation of chemisorbed hydrogen through graphene: A flipping mechanism elucidated. Carbon, 2021, 178, 718-727.	5.4	10
42	The intermolecular potential of O2â€“O2 in its quintet state: An ab initio study. Chemical Physics Letters, 2005, 414, 11-16.	1.2	9
43	Can density functional theory methods be used to simulate the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si12.gif" overflow="scroll"><mml:mrow><mml:mi>â^Š</mml:mi></mml:mrow></mml:math> phase of solid oxygen?. Chemical Physics Letters, 2014, 592, 170-174.	1.2	9
44	Theoretical evidence for the reaction O2(Î½) + O2(Î½ = 0) â†' O3(X1A1) + O(3P). Chemical Physics Letters, 1997, 276, 152-156.	1.2	8
45	Cyclic Allenes or Diradicals in the Cyclization Reactions of Dienynes Generated by Photolysis of Alkynylcyclohexadienones. Journal of Organic Chemistry, 2000, 65, 5207-5211.	1.7	8
46	A theoretical study on electronic predissociation in the NeBr2 van der Waals molecule. Chemical Physics, 2012, 399, 86-93.	0.9	8
47	The interaction potential of NO-H2 in ground and A Rydberg state. Chemical Physics Letters, 2016, 658, 176-181.	1.2	8
48	Antiferromagnetic vs. non-magnetic Îµ phase of solid oxygen. Periodic density functional theory studies using a localized atomic basis set and the role of exact exchange. Physical Chemistry Chemical Physics, 2017, 19, 2826-2833.	1.3	8
49	On the role of the vibrational dependence of the intermolecular potential in O2(v)+ O2Collisions. Molecular Physics, 2004, 102, 2323-2334.	0.8	7
50	An ab Initio Calculation of the Valence Excitation Spectrum of H₂OÂ·Â·Â·Cl₂: Comparison to Condensed Phase Spectra. Journal of Physical Chemistry A, 2009, 113, 7563-7569.	1.1	7
51	Communications: A model study on the electronic predissociation of the NeBr2 van der Waals complex. Journal of Chemical Physics, 2010, 132, 221103.	1.2	7
52	Density-Difference-Driven Optimized Embedding Potential Method To Study the Spectroscopy of Br₂ in Water Clusters. Journal of Chemical Theory and Computation, 2015, 11, 1155-1164.	2.3	6
53	Nature of the valence excited states of bromine in the T and P clathrate cages. Journal of Chemical Physics, 2017, 146, 144311.	1.2	6
54	Nature of the guest-host interactions for dibromine in the T, P, and H clathrate cages. Journal of Chemical Physics, 2017, 147, 154301.	1.2	6

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55	Halogen Bonding and Cooperative Effects in Chlorine Clathrate: Ab Initio Periodic Study. Journal of Physical Chemistry C, 2019, 123, 24793-24806.	1.5	6
56	A New ab Initio Potential Energy Surface for Studying Vibrational Relaxation in NO(v) + NO Collisions. Journal of Physical Chemistry A, 2011, 115, 2892-2899.	1.1	5
57	Communication: Ab initio study of O4H+: A tracer molecule in the interstellar medium?. Journal of Chemical Physics, 2014, 141, 081101.	1.2	5
58	Ab initio study of the O₄H⁺ novel species: spectroscopic fingerprints to aid its observation. Physical Chemistry Chemical Physics, 2015, 17, 16023-16032.	1.3	5
59	An unrestricted approach for the accurate calculation of the interaction potentials of open-shell monomers: The case of O2â€“O2. Journal of Chemical Physics, 2020, 152, 184304.	1.2	5
60	Single-electron capture cross section in 1-500 keV H+-Mg collisions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 769-775.	0.6	4
61	On the Local Relaxation of Solid Neon upon Rydberg Excitation of a NO Impurity: The Role of the NO(A)âˆ’Ne Interaction Potential and Zero-Point Quantum Delocalization. Journal of Physical Chemistry A, 2009, 113, 14399-14406.	1.1	4
62	Theoretical study of the agostic bond in Me₂Al(tBu₂pz)₂Li(THF). International Journal of Quantum Chemistry, 2012, 112, 3630-3636.	1.0	4
63	Fragmentation dynamics of NOâ€“NO dimer: A quasiclassical dynamics study. Chemical Physics Letters, 2013, 563, 20-24.	1.2	4
64	Experimental and theoretical investigations of single-electron capture and loss in He+-Ar collisions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 3751-3761.	0.6	2
65	Density Functional Study on the Fundamental and Valence Excited States of Dibromine in T, P, and H Clathrate Cages. Journal of Physical Chemistry A, 2020, 124, 7692-7709.	1.1	2
66	Ground state analytical ab initio intermolecular potential for the Cl2-water system. Journal of Chemical Physics, 2015, 142, 144310.	1.2	1
67	An unrestricted approach for the accurate calculation of the intermolecular potential of (O2)4: Implications for the solid epsilon phase. Journal of Chemical Physics, 2021, 154, 104307.	1.2	1
68	From gas phase to condensed phases: The mutable behavior of the Br2-water interaction. , 2021, , 235-265.		1
69	Towards an Accurate Model for Halogens in Aqueous Solutions. Challenges and Advances in Computational Chemistry and Physics, 2015, , 253-274.	0.6	1
70	Core excitations of the solid oxygen Îµ phase: periodicÂhybrid density functional theory studies with localized atomic basis. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	0
71	Halogen bonding and rotational disorder in chlorine clathrate hydrate cages. Journal of Chemical Physics, 2022, 156, 124302.	1.2	0