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	Halogen bonding and rotational disorder in chlorine clathrate hydrate cages. Journal of Chemical Physics, 2022, 156, 124302.	1.2	0
2	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
3	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
4	Permeation of chemisorbed hydrogen through graphene: A flipping mechanism elucidated. Carbon, 2021, 178, 718-727.	5.4	10
5	From gas phase to condensed phases: The mutable behavior of the Br2-water interaction. , 2021, , 235-265.		1
6	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
7	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
8	Halogen Bonding and Cooperative Effects in Chlorine Clathrate: Ab Initio Periodic Study. Journal of Physical Chemistry C, 2019, 123, 24793-24806.	1.5	6
9	Graphene multi-protonation: A cooperative mechanism for proton permeation. Carbon, 2019, 144, 724-730.	5.4	25
10	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
11	Halogen Bonds in Clathrate Cages: A Real Space Perspective. ChemPhysChem, 2018, 19, 2512-2517.	1.0	20
12	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
13	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
14	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
15	Communication: Evidence of halogen bonds in clathrate cages. Journal of Chemical Physics, 2016, 145, 161104.	1.2	17
16	The interaction potential of NO-H2 in ground and A Rydberg state. Chemical Physics Letters, 2016, 658, 176-181.	1.2	8
17	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
18	Ground state analytical ab initio intermolecular potential for the Cl2-water system. Journal of Chemical Physics, 2015, 142, 144310.	1.2	1

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	Towards an Accurate Model for Halogens in Aqueous Solutions. Challenges and Advances in Computational Chemistry and Physics, 2015, , 253-274.	0.6	1
24	Communication: Ab initio study of O4H+: A tracer molecule in the interstellar medium?. Journal of Chemical Physics, 2014, 141, 081101.	1.2	5
25	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
26	Fragmentation dynamics of NOâ€“NO dimer: A quasiclassical dynamics study. Chemical Physics Letters, 2013, 563, 20-24.	1.2	4
27	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
28	Ab initiorovibrational structure of the lowest singlet state of O2-O2. Journal of Chemical Physics, 2012, 137, 114304.	1.2	11
29	Theoretical study of the agostic bond in Me₂Al(tBu₂pz)₂Li(THF). International Journal of Quantum Chemistry, 2012, 112, 3630-3636.	1.0	4
30	Properties of the molecular oxygen trimer from pairwise additive interactions. Chemical Physics, 2012, 399, 80-85.	0.9	10
31	A theoretical study on electronic predissociation in the NeBr2 van der Waals molecule. Chemical Physics, 2012, 399, 86-93.	0.9	8
32	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
33	Molecular oxygen tetramer (O2)4: Intermolecular interactions and implications for theÎµsolid phase. Physical Review B, 2011, 84, .	1.1	25
34	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
35	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
36	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

#	Article	IF	Citations
37	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
38	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
39	On the Local Relaxation of Solid Neon upon Rydberg Excitation of a NO Impurity: The Role of the NO(A)â^Ne Interaction Potential and Zero-Point Quantum Delocalization. Journal of Physical Chemistry A, 2009, 113, 14399-14406.	1.1	4
40	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
41	An ab Initio Calculation of the Valence Excitation Spectrum of H₂OÂ·Â·Cl₂: Comparison to Condensed Phase Spectra. Journal of Physical Chemistry A, 2009, 113, 7563-7569.	1.1	7
42	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
43	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
44	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
45	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
46	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
47	Spin-orbit coupling in O2(v)+O2 collisions. II. Quantum scattering calculations on dimer states involving the XÎ£gâ^'3, a1"g1, and bÎ£g+1 states of O2. Journal of Chemical Physics, 2007, 126, 194309.	1.2	11
48	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/xml/	1.2	20
49	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
50	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
51	The intermolecular potential of NO(A2Î£)â€“Ne: An ab initio study. Chemical Physics Letters, 2006, 421, 389-394.	1.2	26
52	The intermolecular potential of O2â€“O2 in its quintet state: An ab initio study. Chemical Physics Letters, 2005, 414, 11-16.	1.2	9
53	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
54	Electronic excited-state mixing in NeCl2. Journal of Chemical Physics, 2005, 123, 161102.	1.2	11

#	Article	IF	Citations
55	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
56	On the role of the vibrational dependence of the intermolecular potential in O2(v)+ O2Collisions. Molecular Physics, 2004, 102, 2323-2334.	0.8	7
57	Systematic ab initio calculations on the energetics and stability of covalent O4. Journal of Chemical Physics, 2004, 120, 10084-10088.	1.2	15
58	Spinâ€“orbit coupling in O2(v)+O2 collisions: A new energy transfer mechanism. Journal of Chemical Physics, 2004, 120, 10355-10358.	1.2	11
59	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
60	Does ozone have a barrier to dissociation and recombination?. Chemical Physics Letters, 2002, 355, 478-482.	1.2	44
61	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
62	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
63	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
64	Reactivity and electronic states of O4 along minimum energy paths. Journal of Chemical Physics, 2000, 113, 4139-4145.	1.2	45
65	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
66	Title is missing!. Topics in Catalysis, 1998, 6, 163-168.	1.3	20
67	Jump in depletion rates of highly excited O2: reaction or enhanced vibrational relaxation?. Chemical Physics Letters, 1998, 289, 150-155.	1.2	29
68	Potential Energy Surface of the C3H9+Cations. Protonated Propane. Journal of the American Chemical Society, 1998, 120, 3213-3219.	6.6	49
69	Protonated Isobutane. A Theoretical ab Initio Study of the Isobutonium Cations. Journal of the American Chemical Society, 1997, 119, 5193-5199.	6.6	56
70	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
71	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