Ãlvaro ValdÃ©s

List of Publications by Year
in descending order

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56	944	394286	454834
papers	citations	19	30
		h-index	g-index

56	56	56	788
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unraveling the Origin of Symmetry Breaking in H₂O@C₆₀ Endofullerene Through Quantum Computations. ChemPhysChem, 2022, 23, e202200034.	1.0	6
2	Exploring CO₂@sI Clathrate Hydrates as CO₂ Storage Agents by Computational Density Functional Approaches. ChemPhysChem, 2021, 22, 359-369.	1.0	11
3	Encapsulation of a Water Molecule inside C₆₀ Fullerene: The Impact of Confinement on Quantum Features. Journal of Chemical Theory and Computation, 2021, 17, 5839-5848.	2.3	16
4	Equality without equity: The gender pay gap at the National University of Colombia. Latin American Economic Review, 2021, , 1-30.	0.3	0
5	Structural Stability of the CO₂@sI Hydrate: a Bottomâ€Up Quantum Chemistry Approach on the Guestâ€Cage and Interâ€Cage Interactions. ChemPhysChem, 2020, 21, 2618-2628.	1.0	9
6	The smallest proton-bound dimer H ₅ ⁺ : theoretical progress. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180396.	1.6	1
7	Quantum effects on the stability of the He₅I₂ van der Waals conformers. Journal of Computational Chemistry, 2019, 40, 2200-2206.	1.5	0
8	Fully Coupled Quantum Treatment of Nanoconfined Systems: A Water Molecule inside a Fullerene C60. Journal of Chemical Theory and Computation, 2018, 14, 6521-6531.	2.3	13
9	A Systematic Protocol for Benchmarking Guestâ€“Host Interactions by Firstâ€Principles Computations: Capturing CO₂ in Clathrate Hydrates. Chemistry - A European Journal, 2018, 24, 9353-9363.	1.7	13
10	Preferential stabilization of HeI2 van der Waals isomers: the effect of energetics and temperature. RSC Advances, 2017, 7, 19273-19279.	1.7	4
11	Density-functional approximations on CO₂@sI clathrate hydrate interactions. Journal of Physics: Conference Series, 2017, 875, 112015.	0.3	0
12	Temperature effects on the isomerâ€™s stability of van der Waals clusters. Journal of Physics: Conference Series, 2017, 875, 042011.	0.3	0
13	Temperature Dependence of HeBr₂ Isomersâ€™ Stability through Rovibrational Multiconfiguration Time-Dependent Hartree Calculations. Journal of Physical Chemistry A, 2016, 120, 9458-9464.	1.1	9
14	Quantum vibrational dynamics of the Ar2ICl cluster. European Physical Journal D, 2016, 70, 1.	0.6	3
15	Vibrational Calculations of Higher-Order Weakly Bound Complexes: The He_{3,4}I₂ Cases. Journal of Physical Chemistry A, 2015, 119, 12736-12741.	1.1	2
16	Quantum Dynamics of Carbon Dioxide Encapsulated in the Cages of the sI Clathrate Hydrate: Structural Guest Distributions and Cage Occupation. Journal of Physical Chemistry C, 2015, 119, 3945-3956.	1.5	21
17	Theoretical predictions on the role of the internal H3+ rotation in the IR spectra of the H5+ and D5+ cations. Physical Chemistry Chemical Physics, 2014, 16, 6217.	1.3	9
18	Energetics and Solvation Structure of a Dihalogen Dopant (I₂) in ⁴He Clusters. Journal of Physical Chemistry A, 2014, 118, 6492-6500.	1.1	15

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19	First-principles simulations of vibrational states and spectra for and clusters using multiconfiguration time-dependent Hartree approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 26-33.	2.0	6
20	Spectral simulations and vibrational dynamics of the fluxional H+5 cation and its isotopologues: signatures of the shared-proton motions. Journal of Physics: Conference Series, 2014, 488, 102008.	0.3	0
21	Spectroscopy of weakly-bound complexes in highly excited electronic states: the He-I₂(E³Î_g) ion-pair state. Journal of Physics: Conference Series, 2014, 488, 102007.	0.3	1
22	Theoretical simulations of the vibrational predissociation spectra of $${m{H}} ^{+}_{5}$$ and $${m{D}}^{+}_{5}$$ clusters. Highlights in Theoretical Chemistry, 2014, , 125-131.	0.0	0
23	Theoretical Investigation of the Infrared Spectra of the H₅⁺ and D₅⁺ Cations. Journal of Physical Chemistry A, 2013, 117, 9518-9524.	1.1	24
24	Effect of Transition Metal Dopants on Initial Mass Transport in the Dehydrogenation of NaAlH₄: Density Functional Theory Study. Journal of Physical Chemistry C, 2013, 117, 3-14.	1.5	19
25	Quantum Mechanical Characterization of the He₄ICl Weakly Bound Complex. Journal of Physical Chemistry A, 2013, 117, 7217-7223.	1.1	6
26	Reply to the â€œComment on â€˜An ab initio Study of the E ³Î_g State of the Iodine Moleculeâ€™â€• Journal of Physical Chemistry A, 2013, 117, 790-791.	1.1	1
27	Quantum-dynamics study of the ${m H}_5^+$H5+ cluster: Full dimensional benchmark results on its vibrational states. Journal of Chemical Physics, 2012, 136, 104302.	1.2	26
28	Vibrational dynamics of the ${m H}_5^+$H5+ and its isotopologues from multiconfiguration time-dependent Hartree calculations. Journal of Chemical Physics, 2012, 137, 214308.	1.2	23
29	An ab Initio Study of the E ³Î_g State of the Iodine Molecule. Journal of Physical Chemistry A, 2012, 116, 2366-2370.	1.1	14
30	Theoretical Investigation of the He₄Br₂ Conformers. Journal of Physical Chemistry A, 2012, 116, 7169-7176.	1.1	4
31	Theoretical Investigation of Two H₂ Molecules Inside the Cages of the Structure H Clathrate Hydrate. Journal of Physical Chemistry C, 2012, 116, 21664-21672.	1.5	22
32	Theoretical investigation of the Heâ€“I2(E3Îg) ion-pair state: Ab initio intermolecular potential and vibrational levels. Journal of Chemical Physics, 2012, 137, 034303.	1.2	19
33	HeI₂ interaction potential based on an interpolation scheme. International Journal of Quantum Chemistry, 2012, 112, 2971-2975.	1.0	13
34	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. Physical Chemistry Chemical Physics, 2012, 14, 49-70.	1.3	198
35	Theoretical simulations of the vibrational predissociation spectra of H 5 + and D 5 + clusters. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	10
36	A theoretical characterization of multiple isomers of the He2I2 complex. Chemical Physics, 2012, 399, 39-45.	0.9	12

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37	Translation-rotation energy levels of one H₂molecule inside the small, medium and large cages of the structure H clathrate hydrate. Physical Chemistry Chemical Physics, 2011, 13, 2935-2944.	1.3	13
38	Ab initio characterization of the Neâ€“I2 van der Waals complex: Intermolecular potentials and vibrational bound states. Journal of Chemical Physics, 2011, 134, 214304.	1.2	24
39	Theoretical characterization of intermolecular vibrational states through the multi-configuration time dependent Hartree approach: The He2.3ICl clusters. Journal of Chemical Physics, 2011, 135, 244309.	1.2	9
40	Infrared spectrum of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub><mml:msup><mml:mrow /><mml:mo>+</mml:mo></mml:msup></mml:mrow></mml:math>and D<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub><mml:msup>	1.0	19
41	Full-dimensional multi configuration time dependent Hartree calculations of the ground and vibrationally excited states of He2,3Br2 clusters. Journal of Chemical Physics, 2011, 135, 054303.	1.2	9
42	Towards an understanding of the vibrational mode specificity for dissociative chemisorption of CH4 on Ni(111): a 15 dimensional study. Physical Chemistry Chemical Physics, 2010, 12, 7654.	1.3	36
43	Intermolecular Ab Initio Potential and Spectroscopy of the Ground State of HeI₂ Complex Revisited. Journal of Physical Chemistry A, 2009, 113, 5754-5762.	1.1	40
44	HeI[sub 2] Van der Waals Complex: Ab initio Ground and Electronic Excited Potential Surfaces for Studying Dynamics. , 2009, , .		1
45	Ab initiointeraction potentials for X and B excited states of Heâ€“I2for studying dynamics. Journal of Physics: Conference Series, 2009, 194, 122001.	0.3	0
46	Ab initio potential energy surface and spectrum of the B(Î3) state of the HeI2 complex. Journal of Chemical Physics, 2007, 126, 204301.	1.2	31
47	Ab initio vibrational predissociation dynamics of Heâ€“I2(B) complex. Journal of Chemical Physics, 2007, 126, 244314.	1.2	31
48	Additive intermolecular potentials from ab initio calculations: trends in Rg2â€“dihalogen van der Waals trimers. Theoretical Chemistry Accounts, 2007, 118, 511-517.	0.5	14
49	Potential energy surfaces and dynamics of He n Br2 van der Waals complexes. Progress in Theoretical Chemistry and Physics, 2007, , 193-202.	0.2	0
50	A theoretical study of He2ICl van der Waals cluster. Journal of Chemical Physics, 2006, 125, 014313.	1.2	34
51	An overview on potential energy surfaces of rare-gas dihalogen van der Waals clusters. Physica Scripta, 2006, 73, C57-C63.	1.2	13
52	ABINITIO VAN DERWAALS POTENTIAL ENERGYSURFACES APPLICATION TO COMPLEXES OF BROMINE MOLECULE WITH HELIUM ATOMS. , 2006, , 347-369.		0
53	Ab initio calculations, potential representation and vibrational dynamics of He2Br2 van der Waals complex. Journal of Chemical Physics, 2005, 122, 044305.	1.2	36
54	HeBr2complex: ground-state potential and vibrational dynamics fromab initiocalculations. Molecular Physics, 2004, 102, 2277-2283.	0.8	37

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55	Three-Dimensional ab Initio Potential and Ground State Dynamics of the HeI2Complex. Journal of Physical Chemistry A, 2004, 108, 6065-6071.	1.1	36
56	CCSD(T) potential energy surface and bound rovibrational level calculations for the Arâ€“ICl(X) complex. Chemical Physics Letters, 2003, 375, 328-336.	1.2	31