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	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. Physical Chemistry Chemical Physics, 2012, 14, 49-70.	1.3	198
2	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
3	HeBr2complex: ground-state potential and vibrational dynamics fromab initiocalculations. Molecular Physics, 2004, 102, 2277-2283.	0.8	37
4	Three-Dimensional ab Initio Potential and Ground State Dynamics of the HeI2Complex. Journal of Physical Chemistry A, 2004, 108, 6065-6071.	1.1	36
5	Ab initio calculations, potential representation and vibrational dynamics of He2Br2 van der Waals complex. Journal of Chemical Physics, 2005, 122, 044305.	1.2	36
6	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
7	A theoretical study of He2ICl van der Waals cluster. Journal of Chemical Physics, 2006, 125, 014313.	1.2	34
8	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
9	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
10	Ab initio vibrational predissociation dynamics of Heâ€“I2(B) complex. Journal of Chemical Physics, 2007, 126, 244314.	1.2	31
11	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
12	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
13	Theoretical Investigation of the Infrared Spectra of the H₅⁺ and D₅⁺ Cations. Journal of Physical Chemistry A, 2013, 117, 9518-9524.	1.1	24
14	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
15	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
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 Investigation of Two H₂ Molecules Inside the Cages of the Structure H Clathrate Hydrate. Journal of Physical Chemistry C, 2012, 116, 21664-21672.	1.0	19
18	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

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19	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
20	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
21	Energetics and Solvation Structure of a Dihalogen Dopant (I₂) in ⁴He Clusters. Journal of Physical Chemistry A, 2014, 118, 6492-6500.	1.1	15
22	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
23	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
24	An overview on potential energy surfaces of rare-gas dihalogen van der Waals clusters. Physica Scripta, 2006, 73, C57-C63.	1.2	13
25	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
26	HeI₂ interaction potential based on an interpolation scheme. International Journal of Quantum Chemistry, 2012, 112, 2971-2975.	1.0	13
27	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
28	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
29	A theoretical characterization of multiple isomers of the He2I2 complex. Chemical Physics, 2012, 399, 39-45.	0.9	12
30	Exploring CO₂@sI Clathrate Hydrates as CO₂ Storage Agents by Computational Density Functional Approaches. ChemPhysChem, 2021, 22, 359-369.	1.0	11
31	Theoretical simulations of the vibrational predissociation spectra of H 5 + and D 5 + clusters. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	10
32	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
33	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
34	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
35	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
36	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

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37	Quantum Mechanical Characterization of the He₄ICl Weakly Bound Complex. Journal of Physical Chemistry A, 2013, 117, 7217-7223.	1.1	6
38	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
39	Unraveling the Origin of Symmetry Breaking in H₂O@C₆₀ Endofullerene Through Quantum Computations. ChemPhysChem, 2022, 23, e202200034.	1.0	6
40	Theoretical Investigation of the He₄Br₂ Conformers. Journal of Physical Chemistry A, 2012, 116, 7169-7176.	1.1	4
41	Preferential stabilization of HeI2 van der Waals isomers: the effect of energetics and temperature. RSC Advances, 2017, 7, 19273-19279.	1.7	4
42	Quantum vibrational dynamics of the Ar2ICl cluster. European Physical Journal D, 2016, 70, 1.	0.6	3
43	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
44	HeI[sub 2] Van der Waals Complex: Ab initio Ground and Electronic Excited Potential Surfaces for Studying Dynamics. , 2009, , .		1
45	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
46	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
47	The smallest proton-bound dimer H ₅ ⁺ : theoretical progress. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180396.	1.6	1
48	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
49	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
50	Density-functional approximations on CO₂@sI clathrate hydrate interactions. Journal of Physics: Conference Series, 2017, 875, 112015.	0.3	0
51	Temperature effects on the isomerâ€™s stability of van der Waals clusters. Journal of Physics: Conference Series, 2017, 875, 042011.	0.3	0
52	Quantum effects on the stability of the He₅I₂ van der Waals conformers. Journal of Computational Chemistry, 2019, 40, 2200-2206.	1.5	0
53	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
54	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

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55	ABINITIO VAN DERWAALS POTENTIAL ENERGYSURFACES APPLICATION TO COMPLEXES OF BROMINE MOLECULE WITH HELIUM ATOMS. , 2006, , 347-369.		0
56	Equality without equity: The gender pay gap at the National University of Colombia. Latin American Economic Review, 2021, , 1-30.	0.3	0