MarÃ-a Pilar de Lara-Castells

List of Publications by Year
in descending order

90 papers	1,624 citations	257357 24 h-index	377752 34 g-index
92 all docs	92 docs citations	92 times ranked	961 citing authors

#	Article	IF	Citations
1	An inversion technique for the calculation of embedding potentials. Journal of Chemical Physics, 2008, 129, 184104.	1.2	93
2	Theoretical study of the interaction of molecular oxygen with a reduced TiO2 surface. Chemical Physics Letters, 2002, 354, 483-490.	1.2	75
3	Complete basis set extrapolation limit for electronic structure calculations: Energetic and nonenergetic properties of HeBr and HeBr[sub 2] van der Waals dimers. Journal of Chemical Physics, 2001, 115, 10438.	1.2	54
4	Adsorption of Noble-Gas Atoms on the TiO₂(110) Surface: An Ab Initio-Assisted Study with van der Waals-Corrected DFT. Journal of Physical Chemistry C, 2016, 120, 18126-18139.	1.5	51
5	Periodic Hartreeâ€“Fock study of the adsorption of molecular oxygen on a reduced TiO2 (110) surface. Journal of Chemical Physics, 2001, 115, 4798-4810.	1.2	46
6	Theoretical study of the UV-induced desorption of molecular oxygen from the reduced TiO2 (110) surface. Journal of Chemical Physics, 2003, 118, 5098-5105.	1.2	46
7	Role of Boson-Fermion Statistics on the Raman Spectra ofBr2(X)in Helium Clusters. Physical Review Letters, 2004, 93, 053401.	2.9	46
8	The first order contracted density equations: correlation effects.. Advances in Quantum Chemistry, 1998, 31, 37-52.	0.4	45
9	Exploring the Catalytic Properties of Unsupported and TiO₂-Supported Cu₅ Clusters: CO₂ Decomposition to CO and CO₂ Photoactivation. Journal of Physical Chemistry C, 2019, 123, 23064-23074.	1.5	39
10	Communication: Unraveling the 4He droplet-mediated soft-landing from ab initio-assisted and time-resolved density functional simulations: Au@4He300/TiO2(110). Journal of Chemical Physics, 2015, 142, 131101.	1.2	37
11	Energies and density distributions of(He4)Nclusters doped withBr2(X): A Hartree-like approach. Physical Review A, 2005, 71, .	1.0	35
12	Increasing the optical response of TiO₂ and extending it into the visible region through surface activation with highly stable Cu₅ clusters. Journal of Materials Chemistry A, 2019, 7, 7489-7500.	5.2	35
13	Communication: A combined periodic density functional and incremental wave-function-based approach for the dispersion-accounting time-resolved dynamics of 4He nanodroplets on surfaces: 4He/graphene. Journal of Chemical Physics, 2014, 141, 151102.	1.2	34
14	Transferability and accuracy by combining dispersionless density functional and incremental post-Hartree-Fock theories: Noble gases adsorption on coronene/graphene/graphite surfaces. Journal of Chemical Physics, 2015, 143, 194701.	1.2	34
15	Combining density functional and incremental post-Hartree-Fock approaches for van der Waals dominated adsorbate-surface interactions: Ag2/graphene. Journal of Chemical Physics, 2015, 143, 102804.	1.2	34
16	Polar di-halogen molecules solvated in bosonic helium clusters: The paradigm ofICl(X). Physical Review A, 2006, 74, .	1.0	33
17	Helium mediated deposition: Modeling the Heâ‹¯TiO₂(110)-(1Ã—1) interaction potential and application to the collision of a helium droplet from density functional calculations. Journal of Chemical Physics, 2012, 136, 124703.	1.2	31
18	Ab initio design of light absorption through silver atomic cluster decoration of TiO₂. Physical Chemistry Chemical Physics, 2018, 20, 19110-19119.	1.3	31

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19	Assessing the Performance of Dispersionless and Dispersion-Accounting Methods: Helium Interaction with Cluster Models of the TiO₂(110) Surface. Journal of Physical Chemistry A, 2014, 118, 6367-6384.	1.1	30
20	Effects of the Core Location on the Structural Stability of Niâ€“Au Coreâ€“Shell Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 20037-20043.	1.5	28
21	Adsorption and nonadiabatic processes in the photodesorption of molecular oxygen from the reduced TiO2(110) surface. Israel Journal of Chemistry, 2005, 45, 59-76.	1.0	27
22	A full-configuration interaction â€œnuclear orbitalâ€•method to study doped HeN3 clusters (Nâ©½4). Journal of Chemical Physics, 2006, 125, 221101.	1.2	26
23	Exploring the properties of Ag₅â€“TiO₂ interfaces: stable surface polaron formation, UV-Vis optical response, and CO₂ photoactivation. Journal of Materials Chemistry A, 2020, 8, 6842-6853.	5.2	26
24	Raman spectra of (He)N-Br2(X) clusters: The role of boson/fermion statistics in a quantum solvent. Journal of Chemical Physics, 2004, 121, 2975-2984.	1.2	25
25	Quantum Nuclear Motion of Helium and Molecular Nitrogen Clusters in Carbon Nanotubes. Journal of Physical Chemistry C, 2017, 121, 3807-3821.	1.5	25
26	Stability and structure of rare-gas ionic clusters using density functional methods: A study of helium clusters. , 1996, 60, 593-608.		23
27	An optimized full-configuration-interaction nuclear orbital approach to a â€œhard-coreâ€•interaction problem: Application to (H3e)Nâ€“Cl2(B) clusters (Nâ‰¤4). Journal of Chemical Physics, 2009, 131, 194101.	1.2	23
28	The open-shell interaction of He with the Bâ€Š3Îu(0+) state of Br2: Anab initiostudy and its comparison with a diatomics-in-molecule perturbation model. Journal of Chemical Physics, 2004, 120, 2182-2192.	1.2	20
29	Fragmentation of Ar3+ clusters via vibrational predissociation. Chemical Physics Letters, 1995, 242, 336-342.	1.2	19
30	Br2(X) Microsolvation in Helium Clusters: Effect of the Interaction on the Quantum Solvent Density Distribution. ChemPhysChem, 2005, 6, 1348-1356.	1.0	19
31	Argon Interaction with Gold Surfaces: Ab Initio-Assisted Determination of Pair Arâ€“Au Potentials for Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2015, 119, 6897-6908.	1.1	18
32	Carbon Nanotubes Immersed in Superfluid Helium: The Impact of Quantum Confinement on Wetting and Capillary Action. Journal of Physical Chemistry Letters, 2016, 7, 4929-4935.	2.1	18
33	Spatial quenching of a molecular charge-transfer process in a quantum fluid: the Cs_xâ€“C₆₀ reaction in superfluid helium nanodroplets. Physical Chemistry Chemical Physics, 2017, 19, 1342-1351.	1.3	18
34	Helium Droplet-Mediated Deposition and Aggregation of Nanoscale Silver Clusters on Carbon Surfaces. Journal of Physical Chemistry C, 2017, 121, 22248-22257.	1.5	17
35	Accurate ab initio prediction of the rovibrational energy levels and equilibrium geometry of carbonyl selenide (OCSe). Physical Chemistry Chemical Physics, 1999, 1, 3955-3960.	1.3	16
36	Post-Hartree-Fock studies of the He/Mg(0001) interaction: Anti-corrugation, screening, and pairwise additivity. Journal of Chemical Physics, 2016, 144, 244707.	1.2	16

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37	Selective vibrational excitations in the OX (X=F, Cl, Br, I) molecules. Physical Chemistry Chemical Physics, 2000, 2, 1117-1122.	1.3	15
38	Vibrational quenching of CO2(010) by collisions with O(P3) at thermal energies: A quantum-mechanical study. Journal of Chemical Physics, 2006, 124, 164302.	1.2	15
39	Using a Jacobiâ€"Davidson â€œNuclear Orbitalâ€•Method for Small Doped 3 He Clusters. Few-Body Systems, 2009, 45, 233-236.	0.7	15
40	Collective Bosonic Excitations in Doped para-H₂ Clusters through the Full-Configuration-Interaction Nuclear Orbital Approach. Journal of Physical Chemistry Letters, 2011, 2, 2145-2151.	2.1	15
41	Nuclear Bound States of Molecular Hydrogen Physisorbed on Graphene: An Effective Two-Dimensional Model. Journal of Physical Chemistry A, 2015, 119, 11022-11032.	1.1	15
42	Blueshifts of the Bâ†X excitation spectra of He79Br2 using a DIM-based potential. Chemical Physics Letters, 2000, 318, 578-584.	1.2	14
43	Spectral simulations of polar diatomic molecules immersed in He clusters: application to the ICl (X) molecule. Physica Scripta, 2007, 76, C96-C103.	1.2	14
44	Doped helium clusters analyzed through quantum chemistry methods. International Journal of Quantum Chemistry, 2007, 107, 2902-2921.	1.0	14
45	Quantum solvent states and rovibrational spectra of small doped H3e clusters through the full-configuration-interaction nuclear orbital approach: The (H3e)Nâ€"Cl2(X) case (Nâ‰¤4). Journal of Chemical Physics, 2010, 132, 194313.	1.2	14
46	Including nuclear quantum effects into highly correlated electronic structure calculations of weakly bound systems. Journal of Chemical Physics, 2013, 138, 184113.	1.2	14
47	Ag5-induced stabilization of multiple surface polarons on perfect and reduced TiO2 rutile (110). Journal of Chemical Physics, 2020, 153, 164702.	1.2	14
48	Thermally Induced Diffusion and Restructuring of Iron Triade (Fe, Co, Ni) Nanoparticles Passivated by Several Layers of Gold. Journal of Physical Chemistry C, 2020, 124, 16680-16688.	1.5	14
49	Structure and anisotropy of ionic argon clusters using density functional models. Chemical Physics, 1996, 208, 25-34.	0.9	13
50	Exact and quantum chemistry-like calculations in helium doped clusters: The He2Br2(X) example. International Journal of Quantum Chemistry, 2007, 107, 2756-2762.	1.0	13
51	Microscopic description of small doped ³He clusters through the fullâ€configurationâ€interaction nuclear orbital approach: The (³He)_Nâ€Br₂(X) case revisited. International Journal of Quantum Chemistry, 2011, 111, 406-415.	1.0	13
52	First-principles modelling of the new generation of subnanometric metal clusters: Recent case studies. Journal of Colloid and Interface Science, 2022, 612, 737-759.	5.0	13
53	Quantum confinement of molecular deuterium clusters in carbon nanotubes: ab initio evidence for hexagonal close packing. Physical Chemistry Chemical Physics, 2017, 19, 28621-28629.	1.3	12
54	Ab Initio Confirmation of a Harpoon-Type Electron Transfer in a Helium Droplet. Journal of Physical Chemistry Letters, 2017, 8, 4284-4288.	2.1	12

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55	On the Stability of Cu₅ Catalysts in Air Using Multireference Perturbation Theory. Journal of Physical Chemistry C, 2019, 123, 27064-27072.	1.5	12
56	Key role of spinâ€“orbit effects in the relaxation of CO2(010) by thermal collisions with O(3Pj). Molecular Physics, 2007, 105, 1171-1181.	0.8	11
57	A Finite Cluster Approach to an Extended Transition Metal Oxide: A Wave Function Based Study. Journal of Physical Chemistry C, 2011, 115, 17540-17557.	1.5	11
58	Solvent states and spectroscopy of doped helium clusters as a quantum-chemistry-like problem. Physical Chemistry Chemical Physics, 2013, 15, 10126.	1.3	11
59	Physisorption of helium on a TiO2(110) surface: Periodic and finite cluster approaches. Chemical Physics, 2012, 399, 272-280.	0.9	10
60	Model studies of the structure and optical properties of the TiO₂(110) surface with an adsorbed Ag atom. Molecular Physics, 2019, 117, 2267-2274.	0.8	10
61	Exact, Bornâ€“Oppenheimer, and quantum-chemistry-like calculations in helium clusters doped with light molecules: The He2N2(X) system. Journal of Chemical Physics, 2008, 128, 164313.	1.2	9
62	A Path Integral Molecular Dynamics Simulation of a Harpoon-Type Redox Reaction in a Helium Nanodroplet. Molecules, 2021, 26, 5783.	1.7	8
63	Some properties of the lower electronic states for nonlinear He3+ clusters. Journal of Chemical Physics, 1997, 107, 1522-1528.	1.2	7
64	Relevant space within the spin-adapted reduced Hamiltonian theory. I. Study of the BH molecule. International Journal of Quantum Chemistry, 1997, 65, 97-105.	1.0	7
65	Spin-dependent and Coriolis interactions by an improved configuration interaction treatment: predissociation of excited fine structure levels of OH/OD. Molecular Physics, 2000, 98, 1713-1727.	0.8	7
66	Helium and Argon Interactions with Gold Surfaces: Ab Initio-Assisted Determination of the Heâ€“Au Pairwise Potential and Its Application to Accommodation Coefficient Determination. Journal of Physical Chemistry C, 2018, 122, 14606-14614.	1.5	7
67	Computed energy curves for modelling the dissociation of helium trimer ions. Chemical Physics Letters, 1996, 259, 641-646.	1.2	6
68	Mode excitation dynamics in the fragmentation of Ar3+: An helicity decoupling study. Journal of Chemical Physics, 1997, 106, 1718-1728.	1.2	6
69	A full quantum study of the vibrational predissociation mechanisms in Ar3+ cluster. Chemical Physics, 1997, 218, 71-81.	0.9	6
70	Diffusion Monte Carlo description of Cs₂(³Î£_u)â€“(⁴He)_Nclusters: an example of weak dopantâ€“helium interaction. Physica Scripta, 2011, 84, 028107.	1.2	6
71	A nuclear spin and spatial symmetry-adapted full quantum method for light particles inside carbon nanotubes: clusters of ³He, ⁴He, and para-H₂. Physical Chemistry Chemical Physics, 2021, 23, 7908-7918.	1.3	6
72	Nonadiabatic Effects in the Molecular Oxidation of Subnanometric Cu₅ Clusters. Journal of Physical Chemistry A, 2021, 125, 9143-9150.	1.1	6

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73	From Molecular Aggregation to a One-Dimensional Quantum Crystal of Deuterium Inside a Carbon Nanotube of 1 nm Diameter. Journal of Physical Chemistry Letters, 2020, 11, 5081-5086.	2.1	5
74	Spectroscopy of a rotating hydrogen molecule in carbon nanotubes. Physical Chemistry Chemical Physics, 2019, 21, 3423-3430.	1.3	4
75	Computational Characterization of the Intermixing of Iron Triade (Fe, Co, and Ni) Surfaces and Sub-nanometric Clusters with Atomic Gold. ACS Omega, 2021, 6, 16165-16175.	1.6	4
76	Unravelling Coriolis temperature-dependent effects on doped helium clusters: Vib-rotational Raman spectra of (3,4He)4â€“Cl2(X). Chemical Physics Letters, 2013, 555, 12-18.	1.2	3
77	Ab initio modelling of molecular hydrogen rotation in the outside of carbonÂnanotubes. Molecular Physics, 2019, 117, 1746-1757.	0.8	3
78	New tools for the astrochemist: Multi-scale computational modelling and helium droplet-based spectroscopy. Physics of Life Reviews, 2020, 32, 95-98.	1.5	3
79	Mini Review: Quantum Confinement of Atomic and Molecular Clusters in Carbon Nanotubes. Frontiers in Chemistry, 2021, 9, 796890.	1.8	3
80	On a possible mechanism for Ar_4^+ fragmentation. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 41, 211-217.	1.0	2
81	Improving the second order reduced density matrix within the spin-adapted reduced hamiltonian theory. An application to the BeH2 potential curve. Computational and Theoretical Chemistry, 1995, 341, 33-40.	1.5	1
82	Collisional heating in ionic argon clusters The Ar+Ar2+ case. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 901-907.	1.7	1
83	Relevant space within the spin-adapted reduced Hamiltonian theory. II. Study of the ? cloud in benzene and naphthalene. International Journal of Quantum Chemistry, 1997, 65, 107-119.	1.0	1
84	Potential energy surface and bound states of the (X⁴Î£)KRbâ€K complex. International Journal of Quantum Chemistry, 2015, 115, 19-27.	1.0	1
85	Structure and anisotropy of ionic argon clusters using density functional models [Chem. Phys. 208 (1996) 25â€“34]1. Chemical Physics, 1997, 219, 117.	0.9	0
86	A quantum chemistry approach to energies, structures, and spectroscopy of doped helium clusters. , 2012, , .		0
87	A full-configuration-interaction nuclear orbital approach and application for small doped He clusters. , 2015, , .		0
88	Challenges in spectroscopy: accuracy versus interpretation from isolated molecules to condensed phases. Physical Chemistry Chemical Physics, 2019, 21, 3395-3396.	1.3	0
89	STRUCTURE AND DYNAMICS OF VAN DER WAALS COMPLEXES: FROM TRIATOMIC TO MEDIUM SIZE CLUSTERS. , 2006, , .		0
90	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