Ricardo Gargano

List of Publications by Year
in descending order

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113 papers	1,324 citations	361413 20 h-index	526287 27 g-index
113 all docs	113 docs citations	113 times ranked	1010 citing authors

#	Article	IF	Citations
1	Effects of temperature and electric field induced phase transitions on the dynamics of polarons and bipolarons. New Journal of Chemistry, 2013, 37, 2829.	2.8	48
2	Intermolecular interactions of H2S with rare gases from molecular beam scattering in the glory regime and from ab initio calculations. Journal of Chemical Physics, 2006, 125, 133111.	3.0	37
3	Theoretical investigation of carotenoid ultraviolet spectra. International Journal of Quantum Chemistry, 2009, 109, 739-745.	2.0	35
4	A simple program to determine the reaction rate and thermodynamic properties of reacting system. Computational and Theoretical Chemistry, 2003, 639, 167-176.	1.5	34
5	Exciton dissociation and charge carrier recombination processes in organic semiconductors. Journal of Chemical Physics, 2011, 135, 224901.	3.0	34
6	Critical temperature and products of intrachain polaron recombination in conjugated polymers. Physical Chemistry Chemical Physics, 2014, 16, 17072-17080.	2.8	34
7	Carbon dioxide adsorption on doped boron nitride nanotubes. RSC Advances, 2014, 4, 28249-28258.	3.6	34
8	Thermochemistry of molecules in the B/F/H/N system. International Journal of Quantum Chemistry, 2005, 103, 659-684.	2.0	33
9	Theoretical Study of CH4â^'CH4, CHF3â^'CH4, CH4â^'H2O, and CHF3â^'H2O Dimers. Journal of Physical Chemistry A, 2009, 113, 14818-14823.	2.5	30
10	CO₂ adsorption on single-walled boron nitride nanotubes containing vacancy defects. RSC Advances, 2015, 5, 27412-27420.	3.6	28
11	Methanol Solvation Effect on the Proton Rearrangement of Curcuminâ€™s Enol Forms: An Ab Initio Molecular Dynamics and Electronic Structure Viewpoint. Journal of Physical Chemistry C, 2016, 120, 19923-19931.	3.1	27
12	Impurity effects on polaron dynamics in graphene nanoribbons. Carbon, 2015, 91, 171-177.	10.3	26
13	Synthesis, theoretical calculation and anticancer activity of 4,6-diacetylresorcinol-dithiocarbazates and their Copper(II) complexes. Journal of Molecular Structure, 2020, 1212, 128083.	3.6	25
14	Theoretical Temperature Dependence of the Charge-Carrier Mobility in Semiconducting Polymers. Journal of Physical Chemistry A, 2009, 113, 14591-14594.	2.5	24
15	Potential acetylcholinesterase inhibitors: molecular docking, molecular dynamics, and in silico prediction. Journal of Molecular Modeling, 2017, 23, 67.	1.8	24
16	Theoretical study of the reactions BF3+ BX, where X = H or N. International Journal of Quantum Chemistry, 2005, 103, 685-694.	2.0	23
17	Thermal effects on photogeneration of free carriers in organic conductors. Chemical Physics Letters, 2010, 493, 283-287.	2.6	22
18	Polaron Properties in Armchair Graphene Nanoribbons. Journal of Physical Chemistry A, 2016, 120, 4893-4900.	2.5	21

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19	Impurity effects and temperature influence on the exciton dissociation dynamics in conjugated polymers. Chemical Physics Letters, 2013, 580, 108-114.	2.6	20
20	Vibrational and Electronic Structure Analysis of a Carbon Dioxide Interaction with Functionalized Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2013, 117, 2854-2861.	2.5	20
21	Dynamical Study of Impurity Effects on Bipolaronâ€“Bipolaron and Bipolaronâ€“Polaron Scattering in Conjugated Polymers. Journal of Physical Chemistry B, 2013, 117, 11801-11811.	2.6	20
22	Attack angle dependence of the Na+HFâ†'NaF+H reaction at J=0. Chemical Physics Letters, 1999, 309, 257-264.	2.6	19
23	Impact of the Electronâ€“Phonon Interactions on the Polaron Dynamics in Graphene Nanoribbons. Journal of Physical Chemistry A, 2016, 120, 4901-4906.	2.5	19
24	The Na+HF reactive probabilities calculations using two different potential energy surfaces. Chemical Physics Letters, 2002, 361, 271-276.	2.6	18
25	Theoretical rate constants for the reaction BF2+NF=BF3+N of importance in boron nitride chemistry. Chemical Physics Letters, 2005, 413, 151-156.	2.6	18
26	Ab initio studies of hydrogen-bonded complexes: The H2O dimer, trimer and H2OCO. Chemical Physics Letters, 2006, 427, 29-34.	2.6	18
27	Impurity effects on polaron-exciton formation in conjugated polymers. Journal of Chemical Physics, 2013, 139, 174903.	3.0	18
28	A first-principles study of the substitutional doping of the MgCl₂ monolayer for spintronics applications. New Journal of Chemistry, 2020, 44, 8833-8839.	2.8	18
29	Rovibrational energies and spectroscopic constants for H2Oâ^'Ng complexes. Journal of Molecular Modeling, 2014, 20, 2498.	1.8	17
30	A combined crossed molecular beams and theoretical study of the reaction CN+C2H4. Chemical Physics, 2015, 449, 34-42.	1.9	17
31	Fitting potential energy surface for reactive scattering dynamics through generalized simulated annealing. Chemical Physics Letters, 2002, 359, 420-427.	2.6	16
32	Theoretical calculations of a new potential energy surface for the H + Li2 reaction. Chemical Physics Letters, 2010, 490, 123-126.	2.6	16
33	Coupled-cluster based basis sets for valence correlation calculations. Journal of Chemical Physics, 2016, 144, 104106.	3.0	16
34	Complexes of water with the fluoromethanes. Chemical Physics Letters, 2006, 431, 51-55.	2.6	15
35	Molecular Dynamics Investigation of Charge Carrier Density Influence over Mobility in Conjugated Polymers. Journal of Physical Chemistry A, 2009, 113, 14975-14978.	2.5	15
36	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. Chemical Physics Letters, 2013, 555, 168-172.	2.6	15

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37	Fitting potential energy surface of reactive systems via genetic algorithm. International Journal of Quantum Chemistry, 2006, 106, 2650-2657.	2.0	14
38	The H + Li2 bimolecular exchange reaction: Dynamical and kinetical properties at J = 0. Journal of Chemical Physics, 2012, 136, 134319.	3.0	14
39	Methanol, ethanol, propanol, and butanol adsorption on H-ZSM-5 zeolite: an ONIOM study. Journal of Molecular Modeling, 2019, 25, 34.	1.8	14
40	Computational analysis of vibrational frequencies and rovibrational spectroscopic constants of hydrogen sulfide dimer using MP2 and CCSD(T). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118540.	3.9	14
41	Parallel time independent quantum calculations of atom diatom reactivity. Lecture Notes in Computer Science, 1996, , 361-370.	1.3	14
42	A chromophoric study of 2-ethylhexyl p-methoxycinnamate. Chemical Physics Letters, 2011, 516, 162-165.	2.6	13
43	Spectroscopic properties of the molecular ion in the 8kÏ€, 9kÏƒ, 9lÏ€, 9lÏƒ and 10oÏƒ electronic states. Journal of Molecular Spectroscopy, 2012, 273, 26-29.	1.2	13
44	Reactive Scattering between Excitons and Charge Carriers in Conjugated Polymers. Journal of Physical Chemistry C, 2014, 118, 23451-23458.	3.1	13
45	Similarity search combined with docking and molecular dynamics for novel hAChE inhibitor scaffolds. Journal of Molecular Modeling, 2018, 24, 41.	1.8	13
46	Temperature effects on polaron stability in polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2448-2453.	2.0	12
47	Temperature effects on intrachain recombination of bipolarons in conjugated polymers. Chemical Physics Letters, 2014, 614, 151-155.	2.6	12
48	Relativistic Four-Component Potential Energy Curves for the Lowest 23 Covalent States of Molecular Bromine (Br₂). Journal of Physical Chemistry A, 2014, 118, 5818-5822.	2.5	12
49	Discovery of sustainable drugs for Alzheimer's disease: cardanol-derived cholinesterase inhibitors with antioxidant and anti-amyloid properties. RSC Medicinal Chemistry, 2021, 12, 1154-1163.	3.9	11
50	Molecular properties calculations using the qâ€integral method. International Journal of Quantum Chemistry, 2008, 108, 2540-2549.	2.0	10
51	Fully relativistic rovibrational energies and spectroscopic constants of the lowest $$ {ext{X}}:(1)0_g^{ + } $$, Aâ€²:(1)2 u , A:(1)1 u , $$ {ext{B}}prime :(1)0_u^{ - } $$ and $$ {ext{B}}:(1)0_u^{ + } $$ states of molecular chlorine. Journal of Molecular Modeling, 2012, 18, 4343-4348.	1.8	10
52	ONIOM study of dissociated hydrogen and water on ZnO surface. International Journal of Quantum Chemistry, 2012, 112, 3223-3227.	2.0	10
53	4-Component correlated all-electron study on Eka-actinium Fluoride (E121F) including Gaunt interaction: Accurate analytical form, bonding and influence on rovibrational spectra. Chemical Physics Letters, 2016, 662, 169-175.	2.6	10
54	A theoretical study of adsorbed non-metallic atoms on magnesium chloride monolayers. New Journal of Chemistry, 2019, 43, 7778-7783.	2.8	10

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55	A genetic algorithm to build diatomic potentials. Computational and Theoretical Chemistry, 2006, 769, 47-51.	1.5	9
56	Benzeneâ€“kaolinite interaction properties. International Journal of Quantum Chemistry, 2012, 112, 2828-2831.	2.0	9
57	Ab Initio correlated all electron Dirac-Fock calculations for eka-francium fluoride (E119F). Journal of the Brazilian Chemical Society, 2012, 23, 1104-1113.	0.6	9
58	The quantum description (J =0) of the Na+DFâ†'NaF+D isotopic reaction. Computational and Theoretical Chemistry, 2001, 539, 215-222.	1.5	8
59	Calculation of the H₂⁺ rovibrational energies and spectroscopic constants in the 2pÏƒ, 3dÏƒ, 4dÏƒ, 4fÏƒ, 4fÏƒ, 5gÏƒ, and 6iÏƒ electronic states. International Journal of Quantum Chemistry, 2012, 112, 829-833.	2.0	8
60	Rovibrational energy and spectroscopic constant calculations of CH 4â€‰â‹¯â€‰CH 4, CH 4â€‰â‹¯â€‰H 2 O, CH 4â€‰â‹¯â€‰CHF H 2 Oâ€‰â‹¯â€‰CHF 3 dimers. Journal of Molecular Modeling, 2014, 20, 2298.	1.8	8
61	BTEX adsorption on TiO2 anatase and rutile surfaces: DFT functionals. Journal of Molecular Modeling, 2019, 25, 137.	1.8	8
62	A Theoretical Investigation of ZnO Nanotubes: Size and Diameter. Current Physical Chemistry, 2013, 3, 400-407.	0.2	8
63	Quantum Monte Carlo and genetic algorithm study of the potential energy surface of the H molecule. International Journal of Quantum Chemistry, 2008, 108, 2318-2325.	2.0	7
64	Dynamical properties and thermal rate coefficients for the Na + HF reaction using genetic algorithm. International Journal of Quantum Chemistry, 2010, 110, 1070-1079.	2.0	7
65	Theoretical study of tetrahydrofuran: Comparative investigation of spectroscopic and structural properties between gas and liquid phases. International Journal of Quantum Chemistry, 2011, 111, 2914-2921.	2.0	7
66	Supersonic quasi-particles dynamics in organic semiconductors. Chemical Physics Letters, 2012, 550, 146-149.	2.6	7
67	Concentration effects on intrachain polaron recombination in conjugated polymers. Physical Chemistry Chemical Physics, 2015, 17, 1299-1308.	2.8	7
68	Structural, theoretical and biological activity of mono and binuclear nickel(II) complexes with symmetrical and asymmetrical 4,6-diacetylresorcinol-dithiocarbazate ligands. Journal of Inorganic Biochemistry, 2021, 224, 111559.	3.5	7
69	Quantum and classical study of vibrational states of Hâ€‰+2 and Hâ€‰+3 molecules. International Journal of Quantum Chemistry, 2003, 95, 149-152.	2.0	6
70	NF3+N=NF2+NF rate constant calculated using TST with simple tunneling correction. Computational and Theoretical Chemistry, 2006, 769, 201-205.	1.5	6
71	Acetylcholinesterase inhibitors: Modeling potential candidates. International Journal of Quantum Chemistry, 2013, 113, 1461-1466.	2.0	6
72	A Spectroscopic Validation of the Improved Lennardâ€“Jones Model. Molecules, 2021, 26, 3906.	3.8	6

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73	Quasiclassical trajectory calculations of isotopic reactionsNa +XF ?NaF +X (X =D,T andM?) on two different potential energy surfaces. International Journal of Quantum Chemistry, 2003, 95, 159-163.	2.0	5
74	Use of generalized exponential function to build three-dimensional reactive surfaces. Physica A: Statistical Mechanics and Its Applications, 2010, 389, 3604-3612.	2.6	5
75	Thermal rate coefficients calculation for the H⁺ + LiH reaction. International Journal of Quantum Chemistry, 2010, 110, 2024-2028.	2.0	5
76	Molecular modeling of cardanol-derived AChE inhibitors. Chemical Physics Letters, 2019, 731, 136591.	2.6	5
77	Theoretical Investigation on H2O2-Ng (He, Ne, Ar, Kr, Xe, and Rn) Complexes Suitable for Stereodynamics: Interactions and Thermal Chiral Rate Consequences. Frontiers in Chemistry, 2019, 6, 671.	3.6	5
78	Rovibrational energies and spectroscopic constants of the H system in the electronic states 1SÏƒ, 7iÏƒ, 5fÏ€, 5gÏ€, 6iÏ€, and 6iÏ•. International Journal of Quantum Chemistry, 2008, 108, 2398-2402.	2.0	4
79	Thermal Rate Constant Calculation of the NF + F Reactive System Multiple Arrangements. Journal of Physical Chemistry A, 2011, 115, 8248-8254.	2.5	4
80	A detailed reactive cross section study of X + Li2 â†' Li + LiX, with X = H, D, T, and Mu. Journal of Molecular Modeling, 2014, 20, 2315.	1.8	4
81	Krypton-methanol spectroscopic study: Assessment of the complexation dynamics and the role of the van der Waals interaction. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 205, 179-185.	3.9	4
82	Silicon carbide nanobelt: A novel molecule with potential technological application. Computational and Theoretical Chemistry, 2020, 1171, 112645.	2.5	4
83	Hydrogen sulphide <scp>H₂S</scp> and noble gases (Ng = He, Ne, Ar, Kr, Xe, Rn) complexes: A theoretical study of their dynamics, spectroscopy, and interactions. International Journal of Quantum Chemistry, 2020, 120, e26266.	2.0	4
84	Relativistic four-component potential energy curves for the lowest 23 covalent states of molecular astatine (At2). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 245, 118869.	3.9	4
85	Spectroscopy, lifetime, and charge-displacement of the methanol-noble gas complexes: An integrated experimental-theoretical investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 246, 119049.	3.9	4
86	Accurate acid dissociation constant (pKa) calculation for the sulfachloropyridazine and similar molecules. Journal of Molecular Modeling, 2021, 27, 233.	1.8	4
87	Predicting New Pathways for the Reaction CN + C2H2. Revista Virtual De Quimica, 2016, 8, 515-524.	0.4	4
88	Quasi-classical dynamical properties and reaction rate of the Na + HF system on two different potential energy surfaces. International Journal of Quantum Chemistry, 2005, 103, 695-702.	2.0	3
89	Linking model Hamiltonians to ab initio and semiempirical methods in descriptions of impurities in conjugated polymers. International Journal of Quantum Chemistry, 2005, 103, 537-542.	2.0	3
90	Dynamics of photoexcitations with interchain coupling in conjugated polymers. International Journal of Quantum Chemistry, 2008, 108, 2442-2447.	2.0	3

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91	A Computational Investigation of the Multiple Channels of the NF2 + F Reaction. Journal of Physical Chemistry A, 2009, 113, 14336-14342.	2.5	3
92	H₂O₂â€“Ng dynamics predictions using an accurate potential energy surface. Molecular Physics, 0, , 1-6.	1.7	3
93	The interaction of CCl4 with Ng (Ngâ€‰=â€‰He, Ne, Ar), O2, D2O and ND3: rovibrational energies, spectroscopic constants and theoretical calculations. Journal of Molecular Modeling, 2017, 23, 87.	1.8	3
94	A novel analytical potential function for dicationic diatomic molecular systems based on deformed exponential function. Journal of Molecular Modeling, 2017, 23, 182.	1.8	3
95	On the Angular Distribution of the H+Li2 Cross Sections: a Converged Time-Independent Quantum Scattering Study. Scientific Reports, 2018, 8, 1044.	3.3	3
96	CO2 adsorption in nitrogen-doped single-layered graphene quantum dots: a spectroscopic investigation. Journal of Molecular Modeling, 2019, 25, 66.	1.8	3
97	Nature and role of the weak intermolecular bond in enantiomeric conformations of H₂O₂â€“noble gas adducts: a chiral prototypical model. New Journal of Chemistry, 2021, 45, 8240-8247.	2.8	3
98	Investigation of strength and nature of the weak intermolecular bond in NH2 radical-noble gas atom adducts and evaluation of their basic spectroscopic features. Chemical Physics Letters, 2021, 769, 138386.	2.6	3
99	Magnetism and perfect spin filtering in pristine MgCl₂ nanoribbons modulated by edge modification. Physical Chemistry Chemical Physics, 2022, 24, 3370-3378.	2.8	3
100	Functionalized graphene-based Quantum Dots: Promising adsorbents for CO, NO2, SO2, and NH3 Pollutant Gases. Materials Today Communications, 2022, 31, 103426.	1.9	3
101	Chain length effects on nonlinear excitation transitions in transâ€polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2507-2511.	2.0	2
102	Fully Relativistic 4-Components DFT Investigation on Bonding and Dissociation Energy of HgO. Journal of Computational and Theoretical Nanoscience, 2011, 8, 38-42.	0.4	2
103	H₂⁺ dynamical properties in the electronic states 7jÏƒ, 8jÏƒ, 8kÏƒ, 7iÏ€, and 8jp. International Journal of Quantum Chemistry, 2011, 111, 1316-1320.	2.0	2
104	Quantum Monte Carlo with density matrix: potential energy curve derived properties. Journal of Molecular Modeling, 2017, 23, 104.	1.8	2
105	Quantum isotope effects on the H+Li2 reaction. Journal of Molecular Modeling, 2017, 23, 116.	1.8	2
106	Quantum reactive study of a potential energy surface obtained via genetic algorithm. International Journal of Quantum Chemistry, 2008, 108, 2306-2311.	2.0	1
107	An extensive investigation of reactions involved in the nitrogen trifluoride dissociation. New Journal of Chemistry, 2013, 37, 3244.	2.8	1
108	Alternative analytical forms to model diatomic systems based on the deformed exponential function. Journal of Molecular Modeling, 2014, 20, 2297.	1.8	1

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109	Combining electronic properties and virtual screening for the development of new antioxidants: Troloxâ€like compounds as application example. International Journal of Quantum Chemistry, 2020, 120, e26194.	2.0	1
110	Impurity effects on solitons in conjugated polymer linking model hamiltonians and ab initio method descriptions. Computational and Theoretical Chemistry, 2006, 769, 33-37.	1.5	0
111	Electronic structure of vertically coupled double quantum dots: Optimization of basis functions. Chemical Physics Letters, 2010, 494, 228-231.	2.6	0
112	Dynamics and spectroscopy of van der Waals complexes composed of ammonia and noble gases. Journal of Molecular Modeling, 2019, 25, 126.	1.8	0
113	Accurate spectroscopic properties by diffusion quantum Monte Carlo calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 243, 118707.	3.9	0