

Rafael Ramirez

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

135
papers

3,136
citations

31
h-index

48
g-index

139
ext. papers

3,325
ext. citations

3.2
avg, IF

5.28
L-index

#	Paper	IF	Citations
135	Quantum corrections to classical time-correlation functions: hydrogen bonding and anharmonic floppy modes. <i>Journal of Chemical Physics</i> , 2004 , 121, 3973-83	3.9	254
134	Strong covalent bonding between two graphene layers. <i>Physical Review B</i> , 2008 , 77,	3.3	126
133	Anomalous nuclear quantum effects in ice. <i>Physical Review Letters</i> , 2012 , 108, 193003	7.4	104
132	Water dimer diffusion on Pd[111] assisted by an H-bond donor-acceptor tunneling exchange. <i>Physical Review Letters</i> , 2004 , 92, 136104	7.4	96
131	Simple geometric generation of special points in brillouin-zone integrations. Two-dimensional bravais lattices. <i>International Journal of Quantum Chemistry</i> , 1986 , 30, 391-411	2.1	90
130	The use of symmetry in reciprocal space integrations. Asymmetric units and weighting factors for numerical integration procedures in any crystal symmetry. <i>International Journal of Quantum Chemistry</i> , 1988 , 34, 571-594	2.1	83
129	Heat capacity of water: A signature of nuclear quantum effects. <i>Journal of Chemical Physics</i> , 2010 , 132, 046101	3.9	81
128	Oxygen reactivity in vanadium pentoxide: electronic structure and infrared spectroscopy studies. <i>The Journal of Physical Chemistry</i> , 1990 , 94, 8960-8965		75
127	Electron transfer and electronic structure of KCuFeS ₂ . <i>Journal of Alloys and Compounds</i> , 1996 , 234, 40-43;7		64
126	Quantum contributions in the ice phases: the path to a new empirical model for water-TIP4PQ/2005. <i>Journal of Chemical Physics</i> , 2009 , 131, 024506	3.9	57
125	Path-integral molecular dynamics simulation of diamond. <i>Physical Review B</i> , 2006 , 73,	3.3	51
124	Density functional theory study of the interaction of monomeric water with the Ag{111} surface. <i>Physical Review B</i> , 2004 , 69,	3.3	51
123	Structural and thermodynamic properties of diamond: A path-integral Monte Carlo study. <i>Physical Review B</i> , 2000 , 63,	3.3	50
122	Crystal structure and charge-transport properties of N-trimethyltriindole: Novel p-type organic semiconductor single crystals. <i>Organic Electronics</i> , 2009 , 10, 643-652	3.5	49
121	Interstitial oxygen in germanium and silicon. <i>Physical Review B</i> , 1997 , 56, 3820-3833	3.3	48
120	[NbAs ₈] ₃]a Novel Type of Complex and an Unexpected One-Dimensional Chain Structure: [Rb{NbAs ₈ }] ₂] <i>Angewandte Chemie International Edition in English</i> , 1986 , 25, 353-354		46
119	Vibrational properties and diffusion of hydrogen on graphene. <i>Physical Review B</i> , 2009 , 79,	3.3	45

118	Distinct quantum behavior of hydrogen and muonium in crystalline silicon. <i>Physical Review Letters</i> , 1994 , 73, 126-129	7.4	45
117	Isotope effects in ice Ih: a path-integral simulation. <i>Journal of Chemical Physics</i> , 2011 , 134, 094510	3.9	44
116	The Schrödinger formulation of the Feynman path centroid density. <i>Journal of Chemical Physics</i> , 1999 , 111, 3339-3348	3.9	43
115	Quasi-harmonic approximation of thermodynamic properties of ice Ih, II, and III. <i>Journal of Chemical Physics</i> , 2012 , 137, 044502	3.9	41
114	Quantum path integral simulation of isotope effects in the melting temperature of ice Ih. <i>Journal of Chemical Physics</i> , 2010 , 133, 144511	3.9	40
113	Isotope dependence of the lattice parameter of germanium from path-integral Monte Carlo simulations. <i>Physical Review B</i> , 1997 , 56, 237-243	3.3	39
112	Diffusion of hydrogen in graphite: a molecular dynamics simulation. <i>Journal Physics D: Applied Physics</i> , 2010 , 43, 255402	3	36
111	Can gas hydrate structures be described using classical simulations?. <i>Journal of Chemical Physics</i> , 2010 , 132, 114503	3.9	36
110	Path-integral simulation of solids. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 233201	1.8	35
109	Thermodynamic properties of c-Si derived by quantum path-integral Monte Carlo simulations. <i>Physical Review B</i> , 1996 , 53, 9869-9875	3.3	34
108	Path-integral Monte Carlo simulation of hydrogen in crystalline silicon. <i>Physical Review B</i> , 1995 , 51, 16763-16773	3.3	33
107	Kinetic energy of protons in ice Ih and water: A path integral study. <i>Physical Review B</i> , 2011 , 84,	3.3	32
106	Feynman Effective Classical Potential in the Schrödinger Formulation. <i>Physical Review Letters</i> , 1998 , 81, 3303-3306	7.4	31
105	A Crystal Orbital approach for two- and three-dimensional solids on the basis of CNDO/INDO Hamiltonians. Basis equations. <i>International Journal of Quantum Chemistry</i> , 1988 , 34, 47-71	2.1	31
104	Tight-binding approach to the solid-state structure of the complex Zintl-phase Li ₁₂ Si ₇ . <i>Physical Review B</i> , 1984 , 30, 4870-4873	3.3	31
103	Non-Arrhenius relaxation in micromagnetic models of systems with many degrees of freedom. <i>Physical Review B</i> , 1995 , 52, 16034-16040	3.3	30
102	Path-integral simulation of crystalline silicon. <i>Physical Review B</i> , 1993 , 48, 14659-14662	3.3	30
101	Diffusion of muonium and hydrogen in diamond. <i>Physical Review Letters</i> , 2007 , 99, 205504	7.4	27

100	Hydrogen and muonium in diamond: A path-integral molecular dynamics simulation. <i>Physical Review B</i> , 2006 , 73,	3.3	26
99	Phase-Space Formulation of Thermodynamic and Dynamical Properties of Quantum Particles. <i>Physical Review Letters</i> , 1999 , 83, 4456-4459	7.4	26
98	Energetics of cation ordering in the faujasite framework: Monte Carlo simulations. <i>The Journal of Physical Chemistry</i> , 1992 , 96, 2246-2253		26
97	Quantum path-integral study of the phase diagram and isotope effects of neon. <i>Journal of Chemical Physics</i> , 2008 , 129, 204502	3.9	25
96	Quantum effects in graphene monolayers: Path-integral simulations. <i>Journal of Chemical Physics</i> , 2016 , 145, 224701	3.9	25
95	Anharmonic effects in the optical and acoustic bending modes of graphene. <i>Physical Review B</i> , 2016 , 93,	3.3	24
94	Quantum effects on the maximum in density of water as described by the TIP4PQ/2005 model. <i>Journal of Chemical Physics</i> , 2009 , 131, 124518	3.9	24
93	Nuclear quantum effects in calculated NMR shieldings of ethylene; a Feynman path integral $\bar{\bar{b}}$ initio study. <i>Chemical Physics Letters</i> , 2000 , 332, 117-124	2.5	24
92	On the influence of nuclear fluctuations on calculated NMR shieldings of benzene and ethylene: a Feynman path integral $\bar{\bar{b}}$ initio investigation*. <i>International Journal of Quantum Chemistry</i> , 2002 , 86, 280-296	2.1	23
91	Anharmonic effects on the structural and vibrational properties of the ethyl radical: A path integral Monte Carlo study. <i>Journal of Chemical Physics</i> , 2003 , 119, 4328-4338	3.9	23
90	Path integral Monte Carlo simulations for rigid rotors and their application to water. <i>Molecular Physics</i> , 2011 , 109, 149-168	1.7	22
89	Electrons and nuclei of C ₆ H ₆ and C ₆ D ₆ ; a combined Feynman path integral $\bar{\bar{b}}$ initio approach. <i>Chemical Physics</i> , 1998 , 227, 271-300	2.3	22
88	Path integral calculation of free energies: quantum effects on the melting temperature of neon. <i>Journal of Chemical Physics</i> , 2008 , 129, 064110	3.9	22
87	The Electronic Structure and the Nature of Chemical Bond of Crystalline Li ₁₂ Si ₇ . A Semiempirical Crystal Orbital (CO) Approach Based on the Self-Consistent-Field (SCF) Approximation in the Hartree-Fock (HF) Scheme Applied to One-Dimensional (1D) Subunits of the Li ₁₂ Si ₇ Solid. <i>Zeitschrift Für Elektrotechnik Und Elektrochemie</i> , 1985 , 89, 465-481		21
86	Thermally Assisted Tunneling of the B-H Complex in Silicon. <i>Physical Review Letters</i> , 1997 , 79, 111-114	7.4	20
85	Path-integral molecular dynamics simulation of 3C ₅ SiC. <i>Physical Review B</i> , 2008 , 77,	3.3	20
84	Quantum delocalization of nuclei and electrons: cyclobutadiene. <i>Chemical Physics Letters</i> , 1996 , 248, 379-385	2.5	20
83	Thermal properties of graphene from path-integral simulations. <i>Journal of Chemical Physics</i> , 2018 , 148, 102302	3.9	19

82	Configurational entropy of hydrogen-disordered ice polymorphs. <i>Journal of Chemical Physics</i> , 2014 , 140, 234502	3.9	19
81	On the influence of vibrational modes and intramolecular isomerization processes on the NMR parameters of bullvalene: A Feynman path integral $\bar{\text{ab}}$ initio investigation. <i>Chemical Physics</i> , 2007 , 342, 1-15	2.3	19
80	Elastic properties and mechanical tension of graphene. <i>Physical Review B</i> , 2017 , 95,	3.3	18
79	Anharmonic phonon energies in rare-gas solids derived by path-integral simulations. <i>Physical Review B</i> , 2005 , 72,	3.3	18
78	Nuclear quantum effects in the electronic structure of C ₂ H ₄ : a combined Feynman path integral $\bar{\text{ab}}$ initio approach. <i>Chemical Physics Letters</i> , 1998 , 291, 44-50	2.5	17
77	Rare-gas solids under pressure: A path-integral Monte Carlo simulation. <i>Physical Review B</i> , 2005 , 71,	3.3	17
76	Electrons and nuclei of ethylene isomers; a Feynman path integral $\bar{\text{ab}}$ initio study. <i>Chemical Physics</i> , 2001 , 264, 371-400	2.3	17
75	Dynamics of the Carbon Nuclei in C ₆₀ Studied by Feynman Path-Integral Quantum Monte Carlo Simulations. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 12401-12408		17
74	Spectral decomposition and Bloch equation of the operators represented by fixed-centroid path integrals. <i>Journal of Chemical Physics</i> , 2000 , 113, 10849-10860	3.9	16
73	Synthesis, Crystal Structure, and Electronic Structure of CsCuFeS ₂ . <i>Journal of Solid State Chemistry</i> , 1996 , 122, 31-35	3.3	16
72	On the delocalization of the C nuclei in the C ₆₀ molecule; a Feynman path-integral Monte Carlo study. <i>Journal of Physics Condensed Matter</i> , 1995 , 7, 4847-4853	1.8	15
71	Statistical thermodynamics of Si,Al ordering in aluminosilicate faujasites. <i>Physical Review B</i> , 1992 , 46, 787-794	3.3	15
70	The solid-state electronic structure and the nature of the chemical bond of the ternary Zintl-phase Li ₈ MgSi ₆ . A tight-binding analysis. <i>Chemical Physics</i> , 1985 , 95, 17-35	2.3	15
69	Configurational entropy of ice from thermodynamic integration. <i>Chemical Physics Letters</i> , 2013 , 568-569, 70-74	2.5	14
68	Simulation of quantum zero-point effects in water using a frequency-dependent thermostat. <i>Physical Review B</i> , 2013 , 87,	3.3	14
67	All-quantum description of molecules: electrons and nuclei of C ₆ H ₆ . <i>Chemical Physics Letters</i> , 1997 , 275, 377-385	2.5	14
66	Feynman path integral $\bar{\text{ab}}$ initio investigation of the excited state properties of C ₂ H ₄ . <i>Chemical Physics Letters</i> , 2000 , 322, 527-535	2.5	14
65	Ice and water droplets on graphite: a comparison of quantum and classical simulations. <i>Journal of Chemical Physics</i> , 2014 , 141, 204701	3.9	13

64	Molecular hydrogen in graphite: A path-integral simulation. <i>Physical Review B</i> , 2010 , 82,	3.3	13
63	The phase diagram of ice Ih, II, and III: a quasi-harmonic study. <i>Journal of Chemical Physics</i> , 2012 , 137, 134503	3.9	13
62	An efficient technique for the evaluation of lattice sums in crystal orbital (CO) calculations. <i>Physica Status Solidi (B): Basic Research</i> , 1986 , 135, 661-667	1.3	13
61	Path-integral simulation of ice Ih: The effect of pressure. <i>Physical Review B</i> , 2011 , 84,	3.3	12
60	High-density amorphous ice: a path-integral simulation. <i>Journal of Chemical Physics</i> , 2012 , 137, 104505	3.9	12
59	Finite-temperature properties of the muonium substituted ethyl radical CH ₂ MuCH ₂ : nuclear degrees of freedom and hyperfine splitting constants. <i>Molecular Physics</i> , 2005 , 103, 2407-2436	1.7	12
58	On the validity of formal electron counting rules in lithium silicides. <i>Journal of Physics and Chemistry of Solids</i> , 1987 , 48, 51-56	3.9	12
57	The phase diagram of ice: a quasi-harmonic study based on a flexible water model. <i>Journal of Chemical Physics</i> , 2013 , 139, 084503	3.9	11
56	Low-energy quantum dynamics of atoms at defects; interstitial oxygen in silicon. <i>Journal of Physics Condensed Matter</i> , 1997 , 9, 3107-3116	1.8	11
55	Electron transfer in the insertion of alkali metals in chalcopyrite. <i>Materials Research Bulletin</i> , 1995 , 30, 43-48	5.1	11
54	Microscopic structure and reorientation kinetics of B-H complexes in silicon. <i>Physical Review B</i> , 1997 , 56, 15139-15150	3.3	10
53	Nuclear quantum effects in calculated NMR shieldings of benzene; a Feynman path integral study. <i>Molecular Physics</i> , 2001 , 99, 1155-1158	1.7	10
52	Long- versus short-range Si, Al ordering in zeolites X and Y. <i>Chemical Physics Letters</i> , 1991 , 183, 199-203	2.5	10
51	Molecular dynamics simulation of Xe diffusion on the Si(100)-2 \times 1 surface. <i>Journal of Chemical Physics</i> , 1992 , 96, 7838-7847	3.9	10
50	Ground state and excited state properties of ethylene isomers studied by a combined Feynman path integral-ab initio approach. <i>Molecular Physics</i> , 2001 , 99, 1249-1273	1.7	9
49	The band structure of Ni(H ₅ C ₃ B ₂). An example for energetic stabilization due to dimerization. <i>Chemical Physics</i> , 1986 , 106, 213-224	2.3	9
48	Thermal properties of graphene under tensile stress. <i>Physical Review B</i> , 2018 , 97,	3.3	9
47	Path-integral simulation of ice VII: Pressure and temperature effects. <i>Chemical Physics</i> , 2015 , 461, 125-136		8

46	Topological characterization of crystalline ice structures from coordination sequences. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 16676-85	3.6	8
45	Isotope effects on the lattice parameter of cubic SiC. <i>Physical Review B</i> , 2009 , 79,	3.3	8
44	Dynamics of quantum particles by path-integral centroid simulations: The symmetric Eckart barrier. <i>Journal of Chemical Physics</i> , 1997 , 107, 3550-3557	3.9	8
43	Excited State Properties of C ₆ H ₆ and C ₆ D ₆ Studied by Feynman Path Integral Ab Initio Simulations. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 3169-3180	2.8	8
42	On the relaxation of simple magnetic systems. <i>Journal of Applied Physics</i> , 1996 , 79, 6479	2.5	8
41	The band structure of one-dimensional (tetrazaporphyrinato)cobalt(II). A semi-empirical self-consistent field crystal orbital analysis. <i>Chemical Physics</i> , 1987 , 117, 405-413	2.3	8
40	Synthesis and Crystal Structure of Ba ₆ Cu ₁₂ Fe ₁₃ S ₂₇ . <i>Journal of Solid State Chemistry</i> , 1997 , 128, 62-65	3.3	7
39	Influence of nuclear fluctuations on the NMR parameters of bullvalene: A Feynman path integral Ab initio study. <i>Chemical Physics Letters</i> , 2006 , 432, 579-584	2.5	7
38	Isotope Effect in the Mott Transition; a Prediction on the Basis of Molecular All-Quantum Simulations. <i>Physica Status Solidi (B): Basic Research</i> , 2000 , 219, 313-321	1.3	7
37	The two-dimensional band structure of (polyphthalocyaninato)Ni(II). <i>International Journal of Quantum Chemistry</i> , 1988 , 34, 73-84	2.1	7
36	Thermodynamic properties of graphene bilayers. <i>Physical Review B</i> , 2020 , 101,	3.3	6
35	Feynman path integral Ab initio study of the isotropic hyperfine coupling constants of the muonium substituted ethyl radical CH ₂ MuCH ₂ . <i>Chemical Physics Letters</i> , 2005 , 402, 346-351	2.5	6
34	Addendum to Isotope Effect in the Mott Transition: A Prediction on the Basis of Molecular All-Quantum Simulations. <i>Physica Status Solidi (B): Basic Research</i> , 2000 , 220, 1033-1035	1.3	6
33	The isotope effect in electronic expectation values: an all-quantum study of C ₆ H ₆ and C ₆ D ₆ . <i>Molecular Physics</i> , 1998 , 93, 801-807	1.7	6
32	Molecular hydrogen in silicon: A path-integral simulation. <i>Physical Review B</i> , 2009 , 80,	3.3	5
31	Nuclear degrees of freedom in calculated isotropic hyperfine coupling constants of the ethyl radical: a Feynman path integral Ab initio study. <i>Chemical Physics Letters</i> , 2004 , 389, 367-372	2.5	5
30	The One-Dimensional Band Structure of (Tetrazaporphyrinato)iron(II). <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1987 , 91, 717-724		5
29	Phonon dispersion in two-dimensional solids from atomic probability distributions. <i>Journal of Chemical Physics</i> , 2019 , 151, 224107	3.9	5

28	Nuclear quantum effects in graphene bilayers. <i>Journal of Chemical Physics</i> , 2019 , 150, 204707	3.9	4
27	Anharmonicity of the acoustic modes of graphene. <i>Physical Review B</i> , 2020 , 101,	3.3	4
26	Path-integral simulation of graphene monolayers under tensile stress. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 31898-31909	3.6	4
25	Bond-centred hydrogen and muonium in silicon; a Feynman path-integral simulation. <i>Journal of Physics Condensed Matter</i> , 1996 , 8, 8309-8320	1.8	4
24	Theoretical study of the nuclear degrees of freedom in the isotropic and anisotropic hyperfine coupling constants of the C ₂ H ₅ radical: a Feynman path integral density functional approach. <i>Molecular Physics</i> , 2005 , 103, 105-127	1.7	4
23	Ramírez and López-Ciudad Reply:. <i>Physical Review Letters</i> , 2002 , 88,	7.4	4
22	From metastable to stable states in a magnetic system with many degrees of freedom. <i>Journal of Magnetism and Magnetic Materials</i> , 1995 , 140-144, 1847-1848	2.8	4
21	Modelling the time dependence of the magnetization in a system with many degrees of freedom. <i>Journal of Magnetism and Magnetic Materials</i> , 1996 , 157-158, 363-365	2.8	4
20	Low-temperature delocalization of hydrogen in crystalline silicon. <i>Solid State Communications</i> , 1996 , 97, 319-322	1.6	4
19	Ordering of transition metal atoms in M ₂ CuFeS ₂ (M = Li, Na): electronic structure and Monte Carlo simulations. <i>Chemical Physics</i> , 1994 , 189, 585-591	2.3	4
18	Configurational density of states in zeolite frameworks: a Monte Carlo approach. <i>Chemical Physics Letters</i> , 1992 , 194, 79-83	2.5	4
17	Isotope dependence of dispersion forces: a Feynman path integral ab initio study. <i>Computational and Theoretical Chemistry</i> , 2001 , 536, 277-287		3
16	Feynman path integral - ab initio investigation of the excited-state properties of benzene. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2002 , 35, 2583-2592	1.3	3
15	Defect-mediated melting of Xe adsorbed on the Si(100)-2 x 1 surface: A molecular-dynamics study. <i>Physical Review B</i> , 1993 , 47, 4555-4562	3.3	3
14	Isotopic effects in structural properties of graphene. <i>European Physical Journal B</i> , 2020 , 93, 1	1.2	3
13	Thermal control of graphene morphology: A signature of its intrinsic surface tension. <i>Physical Review B</i> , 2018 , 97,	3.3	2
12	The isotope effect in electronic expectation values: an all-quantum study of C ₆ H ₆ and C ₆ D ₆ . <i>Molecular Physics</i> , 1998 , 93, 801-807	1.7	2
11	Collective demagnetization processes in systems of exchange coupled grains. <i>Journal of Magnetism and Magnetic Materials</i> , 1995 , 140-144, 1843-1844	2.8	2

10	. <i>IEEE Transactions on Magnetics</i> , 1994 , 30, 4359-4361	2	2
9	Commensurate versus incommensurate structure of xenon adsorbed on the Si(100) surface. <i>Surface Science</i> , 1992 , 271, L373-L377	1.8	2
8	Communication: Critical behavior in graphene: Spinodal instability at room temperature. <i>Journal of Chemical Physics</i> , 2018 , 149, 041102	3.9	2
7	Nuclear quantum effects in graphane. <i>Chemical Physics</i> , 2020 , 533, 110737	2.3	1
6	Monte Carlo simulation of Xe adsorbed on Al(100). <i>Surface Science</i> , 1993 , 296, L27-L32	1.8	1
5	Analytic Expressions for the One-Center Elements of Compton Profiles. Slater-Type Orbitals. <i>Physica Status Solidi (B): Basic Research</i> , 1988 , 149, K135-K140	1.3	1
4	Quantum effects in the structural and elastic properties of graphite: Path-integral simulations. <i>Physical Review B</i> , 2021 , 104,	3.3	1
3	Isotopic effects in chair graphane. <i>Journal of Physics and Chemistry of Solids</i> , 2021 , 157, 110182	3.9	0
2	Hydrogen dynamics on defective monolayer graphene. <i>Chemical Physics</i> , 2022 , 111597	2.3	0
1	Comment on A novel approach to calculate thermal expansion of graphene: Molecular dynamics study by Hamid Ghasemi, Ali Rajabpour. <i>European Physical Journal Plus</i> , 2018 , 133, 1	3.1	