Rafael Ramirez

List of Publications by Year in Descending Order

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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	Hydrogen dynamics on defective monolayer graphene. *Chemical Physics*, **2022**, 111597	2.3	0
134	Quantum effects in the structural and elastic properties of graphite: Path-integral simulations. *Physical Review B*, **2021**, 104,	3.3	1
133	Isotopic effects in chair graphane. *Journal of Physics and Chemistry of Solids*, **2021**, 157, 110182	3.9	0
132	Anharmonicity of the acoustic modes of graphene. *Physical Review B*, **2020**, 101,	3.3	4
131	Nuclear quantum effects in graphane. *Chemical Physics*, **2020**, 533, 110737	2.3	1
130	Thermodynamic properties of graphene bilayers. *Physical Review B*, **2020**, 101,	3.3	6
129	Isotopic effects in structural properties of graphene. *European Physical Journal B*, **2020**, 93, 1	1.2	3
128	Nuclear quantum effects in graphene bilayers. *Journal of Chemical Physics*, **2019**, 150, 204707	3.9	4
127	Phonon dispersion in two-dimensional solids from atomic probability distributions. *Journal of Chemical Physics*, **2019**, 151, 224107	3.9	5
126	Thermal properties of graphene from path-integral simulations. *Journal of Chemical Physics*, **2018**, 148, 102302	3.9	19
125	Thermal control of graphene morphology: A signature of its intrinsic surface tension. *Physical Review B*, **2018**, 97,	3.3	2
124	Comment on A novel approach to calculate thermal expansion of graphene: Molecular dynamics study by Hamid Ghasemi, Ali Rajabpour. *European Physical Journal Plus*, **2018**, 133, 1	3.1	
123	Communication: Critical behavior in graphene: Spinodal instability at room temperature. *Journal of Chemical Physics*, **2018**, 149, 041102	3.9	2
122	Thermal properties of graphene under tensile stress. *Physical Review B*, **2018**, 97,	3.3	9
121	Elastic properties and mechanical tension of graphene. *Physical Review B*, **2017**, 95,	3.3	18
120	Path-integral simulation of graphene monolayers under tensile stress. *Physical Chemistry Chemical Physics*, **2017**, 19, 31898-31909	3.6	4
119	Anharmonic effects in the optical and acoustic bending modes of graphene. *Physical Review B*, **2016**, 93,	3.3	24

118	Quantum effects in graphene monolayers: Path-integral simulations. *Journal of Chemical Physics*, **2016**, 145, 224701	3.9	25
117	Path-integral simulation of ice VII: Pressure and temperature effects. *Chemical Physics*, **2015**, 461, 125-136	2.3	8
116	Path-integral simulation of solids. *Journal of Physics Condensed Matter*, **2014**, 26, 233201	1.8	35
115	Ice and water droplets on graphite: a comparison of quantum and classical simulations. *Journal of Chemical Physics*, **2014**, 141, 204701	3.9	13
114	Configurational entropy of hydrogen-disordered ice polymorphs. *Journal of Chemical Physics*, **2014**, 140, 234502	3.9	19
113	Configurational entropy of ice from thermodynamic integration. *Chemical Physics Letters*, **2013**, 568-569, 70-74	2.5	14
112	Topological characterization of crystalline ice structures from coordination sequences. *Physical Chemistry Chemical Physics*, **2013**, 15, 16676-85	3.6	8
111	The phase diagram of ice: a quasi-harmonic study based on a flexible water model. *Journal of Chemical Physics*, **2013**, 139, 084503	3.9	11
110	Simulation of quantum zero-point effects in water using a frequency-dependent thermostat. *Physical Review B*, **2013**, 87,	3.3	14
109	Anomalous nuclear quantum effects in ice. *Physical Review Letters*, **2012**, 108, 193003	7.4	104
108	Quasi-harmonic approximation of thermodynamic properties of ice Ih, II, and III. *Journal of Chemical Physics*, **2012**, 137, 044502	3.9	41
107	High-density amorphous ice: a path-integral simulation. *Journal of Chemical Physics*, **2012**, 137, 104505	3.9	12
106	The phase diagram of ice Ih, II, and III: a quasi-harmonic study. *Journal of Chemical Physics*, **2012**, 137, 134503	3.9	13
105	Path-integral simulation of ice Ih: The effect of pressure. *Physical Review B*, **2011**, 84,	3.3	12
104	Kinetic energy of protons in ice Ih and water: A path integral study. *Physical Review B*, **2011**, 84,	3.3	32
103	Path integral Monte Carlo simulations for rigid rotors and their application to water. *Molecular Physics*, **2011**, 109, 149-168	1.7	22
102	Isotope effects in ice Ih: a path-integral simulation. *Journal of Chemical Physics*, **2011**, 134, 094510	3.9	44
101	Quantum path integral simulation of isotope effects in the melting temperature of ice Ih. *Journal of Chemical Physics*, **2010**, 133, 144511	3.9	40

100	Diffusion of hydrogen in graphite: a molecular dynamics simulation. *Journal Physics D: Applied Physics*, **2010**, 43, 255402	3	36
99	Molecular hydrogen in graphite: A path-integral simulation. *Physical Review B*, **2010**, 82,	3.3	13
98	Heat capacity of water: A signature of nuclear quantum effects. *Journal of Chemical Physics*, **2010**, 132, 046101	3.9	81
97	Can gas hydrate structures be described using classical simulations?. *Journal of Chemical Physics*, **2010**, 132, 114503	3.9	36
96	Molecular hydrogen in silicon: A path-integral simulation. *Physical Review B*, **2009**, 80,	3.3	5
95	Isotope effects on the lattice parameter of cubic SiC. *Physical Review B*, **2009**, 79,	3.3	8
94	Quantum contributions in the ice phases: the path to a new empirical model for water-TIP4PQ/2005. *Journal of Chemical Physics*, **2009**, 131, 024506	3.9	57
93	Quantum effects on the maximum in density of water as described by the TIP4PQ/2005 model. *Journal of Chemical Physics*, **2009**, 131, 124518	3.9	24
92	Crystal structure and charge-transport properties of N-trimethyltriindole: Novel p-type organic semiconductor single crystals. *Organic Electronics*, **2009**, 10, 643-652	3.5	49
91	Vibrational properties and diffusion of hydrogen on graphene. *Physical Review B*, **2009**, 79,	3.3	45
90	Strong covalent bonding between two graphene layers. *Physical Review B*, **2008**, 77,	3.3	126
89	Path integral calculation of free energies: quantum effects on the melting temperature of neon. *Journal of Chemical Physics*, **2008**, 129, 064110	3.9	22
88	Quantum path-integral study of the phase diagram and isotope effects of neon. *Journal of Chemical Physics*, **2008**, 129, 204502	3.9	25
87	Path-integral molecular dynamics simulation of 3C□SiC. *Physical Review B*, **2008**, 77,	3.3	20
86	On the influence of vibrational modes and intramolecular isomerization processes on the NMR parameters of bullvalene: A Feynman path integral □ab initio investigation. *Chemical Physics*, **2007**, 342, 1-15	2.3	19
85	Diffusion of muonium and hydrogen in diamond. *Physical Review Letters*, **2007**, 99, 205504	7.4	27
84	Path-integral molecular dynamics simulation of diamond. *Physical Review B*, **2006**, 73,	3.3	51
83	Hydrogen and muonium in diamond: A path-integral molecular dynamics simulation. *Physical Review B*, **2006**, 73,	3.3	26

82	Influence of nuclear fluctuations on the NMR parameters of bullvalene: A Feynman path integral Ab initio study. *Chemical Physics Letters*, **2006**, 432, 579-584	2.5	7
81	Finite-temperature properties of the muonium substituted ethyl radical CH2MuCH2: nuclear degrees of freedom and hyperfine splitting constants. *Molecular Physics*, **2005**, 103, 2407-2436	1.7	12
80	Feynman path integral ab initio study of the isotropic hyperfine coupling constants of the muonium substituted ethyl radical CH2MuCH2. *Chemical Physics Letters*, **2005**, 402, 346-351	2.5	6
79	Anharmonic phonon energies in rare-gas solids derived by path-integral simulations. *Physical Review B*, **2005**, 72,	3.3	18
78	Theoretical study of the nuclear degrees of freedom in the isotropic and anisotropic hyperfine coupling constants of the C2H5 radical: a Feynman path integral density functional approach. *Molecular Physics*, **2005**, 103, 105-127	1.7	4
77	Rare-gas solids under pressure: A path-integral Monte Carlo simulation. *Physical Review B*, **2005**, 71,	3.3	17
76	Nuclear degrees of freedom in calculated isotropic hyperfine coupling constants of the ethyl radical: a Feynman path integral ab initio study. *Chemical Physics Letters*, **2004**, 389, 367-372	2.5	5
75	Quantum corrections to classical time-correlation functions: hydrogen bonding and anharmonic floppy modes. *Journal of Chemical Physics*, **2004**, 121, 3973-83	3.9	254
74	Density functional theory study of the interaction of monomeric water with the Ag{111} surface. *Physical Review B*, **2004**, 69,	3.3	51
73	Water dimer diffusion on Pd[111] assisted by an H-bond donor-acceptor tunneling exchange. *Physical Review Letters*, **2004**, 92, 136104	7.4	96
72	Anharmonic effects on the structural and vibrational properties of the ethyl radical: A path integral Monte Carlo study. *Journal of Chemical Physics*, **2003**, 119, 4328-4338	3.9	23
71	On the influence of nuclear fluctuations on calculated NMR shieldings of benzene and ethylene: a Feynman path integral ab initio investigation*. *International Journal of Quantum Chemistry*, **2002**, 86, 280-296	2.1	23
70	Ram ez and L pez-Ciudad Reply:. *Physical Review Letters*, **2002**, 88,	7.4	4
69	Feynman path integral - ab initio investigation of the excited-state properties of benzene. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2002**, 35, 2583-2592	1.3	3
68	Excited State Properties of C6H6 and C6D6 Studied by Feynman Path Integral Ab Initio Simulations. *Journal of Physical Chemistry A*, **2002**, 106, 3169-3180	2.8	8
67	Ground state and excited state properties of ethylene isomers studied by a combined Feynman path integral-ab initio approach. *Molecular Physics*, **2001**, 99, 1249-1273	1.7	9
66	Nuclear quantum effects in calculated NMR shieldings of benzene; a Feynman path integral study. *Molecular Physics*, **2001**, 99, 1155-1158	1.7	10
65	Electrons and nuclei of ethylene isomers; a Feynman path integral ab initio study. *Chemical Physics* , **2001**, 264, 371-400	2.3	17

64	Isotope dependence of dispersion forces: a Feynman path integral ab initio study. *Computational and Theoretical Chemistry*, **2001**, 536, 277-287		3
63	Addendum to Isotope Effect in the Mott Transition: A Prediction on the Basis of Molecular All-Quantum Simulations. *Physica Status Solidi (B): Basic Research*, **2000**, 220, 1033-1035	1.3	6
62	Isotope Effect in the Mott Transition; a Prediction on the Basis of Molecular All-Quantum Simulations. *Physica Status Solidi (B): Basic Research*, **2000**, 219, 313-321	1.3	7
61	Feynman path integral ab initio investigation of the excited state properties of C2H4. *Chemical Physics Letters*, **2000**, 322, 527-535	2.5	14
60	Nuclear quantum effects in calculated NMR shieldings of ethylene; a Feynman path integral ab initio study. *Chemical Physics Letters*, **2000**, 332, 117-124	2.5	24
59	Spectral decomposition and Bloch equation of the operators represented by fixed-centroid path integrals. *Journal of Chemical Physics*, **2000**, 113, 10849-10860	3.9	16
58	Structural and thermodynamic properties of diamond: A path-integral Monte Carlo study. *Physical Review B*, **2000**, 63,	3.3	50
57	Phase-Space Formulation of Thermodynamic and Dynamical Properties of Quantum Particles. *Physical Review Letters*, **1999**, 83, 4456-4459	7.4	26
56	The Schrödinger formulation of the Feynman path centroid density. *Journal of Chemical Physics*, **1999**, 111, 3339-3348	3.9	43
55	Nuclear quantum effects in the electronic structure of C2H4: a combined Feynman path integral ab initio approach. *Chemical Physics Letters*, **1998**, 291, 44-50	2.5	17
54	Electrons and nuclei of C6H6 and C6D6; a combined Feynman path integral ab initio approach. *Chemical Physics*, **1998**, 227, 271-300	2.3	22
53	Feynman Effective Classical Potential in the Schrödinger Formulation. *Physical Review Letters*, **1998**, 81, 3303-3306	7.4	31
52	The isotope effect in electronic expectation values: an all-quantum study of C6 H6 and C6 D6. *Molecular Physics*, **1998**, 93, 801-807	1.7	2
51	The isotope effect in electronic expectation values: an all-quantum study of C6H6 and C6D6. *Molecular Physics*, **1998**, 93, 801-807	1.7	6
50	Low-energy quantum dynamics of atoms at defects; interstitial oxygen in silicon. *Journal of Physics Condensed Matter*, **1997**, 9, 3107-3116	1.8	11
49	Thermally Assisted Tunneling of the B-H Complex in Silicon. *Physical Review Letters*, **1997**, 79, 111-114	7.4	20
48	Microscopic structure and reorientation kinetics of B-H complexes in silicon. *Physical Review B*, **1997**, 56, 15139-15150	3.3	10
47	Interstitial oxygen in germanium and silicon. *Physical Review B*, **1997**, 56, 3820-3833	3.3	48

46	Dynamics of quantum particles by path-integral centroid simulations: The symmetric Eckart barrier. *Journal of Chemical Physics*, **1997**, 107, 3550-3557	3.9	8
45	Isotope dependence of the lattice parameter of germanium from path-integral Monte Carlo simulations. *Physical Review B*, **1997**, 56, 237-243	3.3	39
44	Synthesis and Crystal Structure of Ba6Cu12Fe13S27. *Journal of Solid State Chemistry*, **1997**, 128, 62-65	3.3	7
43	All-quantum description of molecules: electrons and nuclei of C6H6. *Chemical Physics Letters*, **1997**, 275, 377-385	2.5	14
42	Bond-centred hydrogen and muonium in silicon; a Feynman path-integral simulation. *Journal of Physics Condensed Matter*, **1996**, 8, 8309-8320	1.8	4
41	Electron transfer and electronic structure of KCuFeS2. *Journal of Alloys and Compounds*, **1996**, 234, 40-42	5.7	64
40	On the relaxation of simple magnetic systems. *Journal of Applied Physics*, **1996**, 79, 6479	2.5	8
39	Modelling the time dependence of the magnetization in a system with many degrees of freedom. *Journal of Magnetism and Magnetic Materials*, **1996**, 157-158, 363-365	2.8	4
38	Quantum delocalization of nuclei and electrons: cyclobutadiene. *Chemical Physics Letters*, **1996**, 248, 379-385	2.5	20
37	Synthesis, Crystal Structure, and Electronic Structure of CsCuFeS2. *Journal of Solid State Chemistry*, **1996**, 122, 31-35	3.3	16
36	Low-temperature delocalization of hydrogen in crystalline silicon. *Solid State Communications*, **1996** , 97, 319-322	1.6	4
35	Thermodynamic properties of c-Si derived by quantum path-integral Monte Carlo simulations. *Physical Review B*, **1996**, 53, 9869-9875	3.3	34
34	Collective demagnetization processes in systems of exchange coupled grains. *Journal of Magnetism and Magnetic Materials*, **1995**, 140-144, 1843-1844	2.8	2
33	From metastable to stable states in a magnetic system with many degrees of freedom. *Journal of Magnetism and Magnetic Materials*, **1995**, 140-144, 1847-1848	2.8	4
32	Electron transfer in the insertion of alkali metals in chalcopyrite. *Materials Research Bulletin*, **1995**, 30, 43-48	5.1	11
31	Non-Arrhenius relaxation in micromagnetic models of systems with many degrees of freedom. *Physical Review B*, **1995**, 52, 16034-16040	3.3	30
30	Path-integral Monte Carlo simulation of hydrogen in crystalline silicon. *Physical Review B*, **1995**, 51, 16761-16771	3.3	33
29	On the delocalization of the C nuclei in the C60molecule; a Feynman path-integral Monte Carlo study. *Journal of Physics Condensed Matter*, **1995**, 7, 4847-4853	1.8	15

28	Dynamics of the Carbon Nuclei in C60 Studied by Feynman Path-Integral Quantum Monte Carlo Simulations. *The Journal of Physical Chemistry*, **1995**, 99, 12401-12408		17
27	. *IEEE Transactions on Magnetics*, **1994**, 30, 4359-4361	2	2
26	Distinct quantum behavior of hydrogen and muonium in crystalline silicon. *Physical Review Letters*, **1994**, 73, 126-129	7.4	45
25	Ordering of transition metal atoms in MCuFeS2 (M = Li, Na): electronic structure and Monte Carlo simulations. *Chemical Physics*, **1994**, 189, 585-591	2.3	4
24	Monte Carlo simulation of Xe adsorbed on Al(100). *Surface Science*, **1993**, 296, L27-L32	1.8	1
23	Path-integral simulation of crystalline silicon. *Physical Review B*, **1993**, 48, 14659-14662	3.3	30
22	Defect-mediated melting of Xe adsorbed on the Si(100)-2 x 1 surface: A molecular-dynamics study. *Physical Review B*, **1993**, 47, 4555-4562	3.3	3
21	Energetics of cation ordering in the faujasite framework: Monte Carlo simulations. *The Journal of Physical Chemistry*, **1992**, 96, 2246-2253		26
20	Statistical thermodynamics of Si,Al ordering in aluminosilicate faujasites. *Physical Review B*, **1992**, 46, 787-794	3.3	15
19	Molecular dynamics simulation of Xe diffusion on the Si(100)-2□1 surface. *Journal of Chemical Physics*, **1992**, 96, 7838-7847	3.9	10
18	Commensurate versus incommensurate structure of xenon adsorbed on the Si(100)□□1 surface. *Surface Science*, **1992**, 271, L373-L377	1.8	2
17	Configurational density of states in zeolite frameworks: a Monte Carlo approach. *Chemical Physics Letters*, **1992**, 194, 79-83	2.5	4
16	Long- versus short-range Si, Al ordering in zeolites X and Y. *Chemical Physics Letters*, **1991**, 183, 199-203	2.5	10
15	Oxygen reactivity in vanadium pentoxide: electronic structure and infrared spectroscopy studies. *The Journal of Physical Chemistry*, **1990**, 94, 8960-8965		75
14	A Crystal Orbital approach for two- and three-dimensional solids on the basis of CNDO/INDO Hamiltonians. Basis equations. *International Journal of Quantum Chemistry*, **1988**, 34, 47-71	2.1	31
13	The two-dimensional band structure of (polyphthalocyaninato)Ni(II). *International Journal of Quantum Chemistry*, **1988**, 34, 73-84	2.1	7
12	The use of symmetry in reciprocal space integrations. Asymmetric units and weighting factors for numerical integration procedures in any crystal symmetry. *International Journal of Quantum Chemistry*, **1988**, 34, 571-594	2.1	83
11	Analytic Expressions for the One-Center Elements of Compton Profiles. Slater-Type Orbitals. *Physica Status Solidi (B): Basic Research*, **1988**, 149, K135-K140	1.3	1

10	The One-Dimensional Band Structure of (Tetrazaporphyrinato)iron(II). *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1987**, 91, 717-724		5
9	On the validity of formal electron counting rules in lithium silicides. *Journal of Physics and Chemistry of Solids*, **1987**, 48, 51-56	3.9	12
8	The band structure of one-dimensional (tetrazaporphyrinato)cobalt(II). A semi-empirical self-consistent field crystal orbital analysis. *Chemical Physics*, **1987**, 117, 405-413	2.3	8
7	[NbAs8]3□a Novel Type of Complex and an Unexpected One-Dimensional Chain Structure: [Rb{NbAs8}]2□*Angewandte Chemie International Edition in English*, **1986**, 25, 353-354		46
6	The band structure of Ni(H5C3B2). An example for energetic stabilization due to dimerization. *Chemical Physics*, **1986**, 106, 213-224	2.3	9
5	An efficient technique for the evaluation of lattice sums in crystal orbital (CO) calculations. *Physica Status Solidi (B): Basic Research*, **1986**, 135, 661-667	1.3	13
4	Simple geometric generation of special points in brillouin-zone integrations. Two-dimensional bravais lattices. *International Journal of Quantum Chemistry*, **1986**, 30, 391-411	2.1	90
3	The Electronic Structure and the Nature of Chemical Bond of Crystalline Li12Si7. 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 Li12Si7 Solid. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1985**, 89, 465-481		21
2	The solid-state electronic structure and the nature of the chemical bond of the ternary Zintl-phase Li8MgSi6. A tight-binding analysis. *Chemical Physics*, **1985**, 95, 17-35	2.3	15
1	Tight-binding approach to the solid-state structure of the complex Zintl-phase Li12Si7. *Physical Review B*, **1984**, 30, 4870-4873	3.3	31