Zlatko BaÄiÄ

List of Publications by Year
in descending order

105	3,015	136950	206112
papers	citations	32 h-index	48 g-index

106	106	106	1096
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Intermolecular rovibrational states of the H2Oâ€“CO2 and D2Oâ€“CO2 van der Waals complexes. Journal of Chemical Physics, 2022, 156, 064301.	3.0	5
2	H₂O inside the fullerene C₆₀: Inelastic neutron scattering spectrum from rigorous quantum calculations. Journal of Chemical Physics, 2022, 156, 124101.	3.0	3
3	Enhanced Sampling Path Integral Methods Using Neural Network Potential Energy Surfaces with Application to Diffusion in Hydrogen Hydrates. Advanced Theory and Simulations, 2021, 4, 2000258.	2.8	13
4	HClâ€“H₂O dimer: an accurate full-dimensional potential energy surface and fully coupled quantum calculations of intra- and intermolecular vibrational states and frequency shifts. Physical Chemistry Chemical Physics, 2021, 23, 7101-7114.	2.8	28
5	DClâ€“H₂O, HClâ€“D₂O, and DClâ€“D₂O Dimers: Inter- and Intramolecular Vibrational States and Frequency Shifts from Fully Coupled Quantum Calculations on a Full-Dimensional Neural Network Potential Energy Surface. Journal of Physical Chemistry A, 2021, 125, 6437-6449.	2.5	11
6	HDOâ€“CO Complex: D-Bonded and H-Bonded Isomers and Intra- and Intermolecular Rovibrational States from Full-Dimensional and Fully Coupled Quantum Calculations. Journal of Physical Chemistry A, 2021, 125, 980-989.	2.5	14
7	Flexible water molecule in C60: Intramolecular vibrational frequencies and translation-rotation eigenstates from fully coupled nine-dimensional quantum calculations with small basis sets. Journal of Chemical Physics, 2020, 152, 014108.	3.0	25
8	Light molecules inside the nanocavities of fullerenes and clathrate hydrates: inelastic neutron scattering spectra and the unexpected selection rule from rigorous quantum simulations. International Reviews in Physical Chemistry, 2020, 39, 425-463.	2.3	10
9	H2Oâ€“CO and D2Oâ€“CO complexes: Intra- and intermolecular rovibrational states from full-dimensional and fully coupled quantum calculations. Journal of Chemical Physics, 2020, 153, 074107.	3.0	21
10	Hydrogen Intramolecular Stretch Redshift in the Electrostatic Environment of Type II Clathrate Hydrates from SchrÃ¶dinger Equation Treatment. Applied Sciences (Switzerland), 2020, 10, 8504.	2.5	1
11	Benzeneâ€“H2O and benzeneâ€“HDO: Fully coupled nine-dimensional quantum calculations of flexible H2O/HDO intramolecular vibrational excitations and intermolecular states of the dimers, and their infrared and Raman spectra using compact bases. Journal of Chemical Physics, 2020, 152, 124103.	3.0	13
12	Weakly bound molecular dimers: Intramolecular vibrational fundamentals, overtones, and tunneling splittings from full-dimensional quantum calculations using compact contracted bases of intramolecular and low-energy rigid-monomer intermolecular eigenstates. Journal of Chemical Physics, 2019, 151, 024305.	3.0	28
13	The Endofullerene HF@C60: Inelastic Neutron Scattering Spectra from Quantum Simulations and Experiment, Validity of the Selection Rule, and Symmetry Breaking. Journal of Physical Chemistry Letters, 2019, 10, 5365-5371.	4.6	11
14	Intramolecular stretching vibrational states and frequency shifts of (H2)2 confined inside the large cage of clathrate hydrate from an eight-dimensional quantum treatment using small basis sets. Journal of Chemical Physics, 2019, 151, 124311.	3.0	23
15	H2, HD, and D2 in the small cage of structure II clathrate hydrate: Vibrational frequency shifts from fully coupled quantum six-dimensional calculations of the vibration-translation-rotation eigenstates. Journal of Chemical Physics, 2019, 150, 154303.	3.0	25
16	An open-chain imaginary-time path-integral sampling approach to the calculation of approximate symmetrized quantum time correlation functions. Journal of Chemical Physics, 2018, 148, 102340.	3.0	10
17	The effect of the condensed-phase environment on the vibrational frequency shift of a hydrogen molecule inside clathrate hydrates. Journal of Chemical Physics, 2018, 148, 144304.	3.0	16
18	Precise characterisation of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 137-155.	3.2	1

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19	Molecules in confinement in clusters, quantum solvents and matrices: general discussion. Faraday Discussions, 2018, 212, 569-601.	3.2	4
20	Perspective: Accurate treatment of the quantum dynamics of light molecules inside fullerene cages: Translation-rotation states, spectroscopy, and symmetry breaking. Journal of Chemical Physics, 2018, 149, 100901.	3.0	22
21	Effects of symmetry breaking on the translationâ€“rotation eigenstates of H₂, HF, and H₂O inside the fullerene C₆₀. Faraday Discussions, 2018, 212, 547-567.	3.2	20
22	Electric-dipole-coupled H₂O@C₆₀ dimer: Translation-rotation eigenstates from twelve-dimensional quantum calculations. Journal of Chemical Physics, 2017, 146, 084303.	3.0	22
23	Accurate quantum calculations of translation-rotation eigenstates in electric-dipole-coupled H2O@C60 assemblies. Chemical Physics Letters, 2017, 683, 172-178.	2.6	10
24	Explaining the symmetry breaking observed in the endofullerenes H₂@C₆₀, HF@C₆₀, and H₂O@C₆₀. Physical Chemistry Chemical Physics, 2017, 19, 31274-31283.	2.8	36
25	Translation-rotation states of H2 in C60: New insights from a perturbation-theory treatment. Journal of Chemical Physics, 2016, 145, 084310.	3.0	15
26	Competing quantum effects in the free energy profiles and diffusion rates of hydrogen and deuterium molecules through clathrate hydrates. Physical Chemistry Chemical Physics, 2016, 18, 32169-32177.	2.8	31
27	Communication: Quantum six-dimensional calculations of the coupled translation-rotation eigenstates of H2O@C60. Journal of Chemical Physics, 2016, 144, 201101.	3.0	36
28	Impact of the Condensed-Phase Environment on the Translationâ€“Rotation Eigenstates and Spectra of a Hydrogen Molecule in Clathrate Hydrates. Journal of Physical Chemistry Letters, 2016, 7, 308-313.	4.6	18
29	General Selection Rule in the Inelastic Neutron Scattering Spectroscopy of a Diatomic Molecule Confined Inside a Near-Spherical Nanocavity. Journal of Physical Chemistry Letters, 2015, 6, 3721-3725.	4.6	20
30	The HD molecule in small and medium cages of clathrate hydrates: Quantum dynamics studied by neutron scattering measurements and computation. Journal of Chemical Physics, 2014, 141, 134501.	3.0	16
31	The von Neumann basis in non-Cartesian coordinates: Application to floppy triatomic molecules. Journal of Chemical Physics, 2014, 141, 234106.	3.0	19
32	Efficient Calculation of Free Energy Differences Associated with Isotopic Substitution Using Path-Integral Molecular Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 1440-1453.	5.3	39
33	Translator-Rotator<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Entrapped Inside<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>	7.8	27
34	H2 in solid C60: Coupled translation-rotation eigenstates in the octahedral interstitial site from quantum five-dimensional calculations. Journal of Chemical Physics, 2013, 138, 244707.	3.0	7
35	Tribute to Joel M. Bowman. Journal of Physical Chemistry A, 2013, 117, 6905-6906.	2.5	0
36	Neutron Scattering Measurements and Computation of the Quantum Dynamics of Hydrogen Molecules Trapped in the Small and Large Cages of Clathrate Hydrates. Journal of Physical Chemistry A, 2013, 117, 7314-7326.	2.5	33

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37	HD in C ₆₀ : theoretical prediction of the inelastic neutron scattering spectrum and its temperature dependence. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2013, 371, 20110630.	3.4	22
38	Inelastic neutron scattering spectrum of H2@C60 and its temperature dependence decoded using rigorous quantum calculations and a new selection rule. Journal of Chemical Physics, 2013, 139, 064309.	3.0	29
39	Rigorous quantum treatment of inelastic neutron scattering spectra of a heteronuclear diatomic molecule in a nanocavity: HD in the small cage of structure II clathrate hydrate. Chemical Physics Letters, 2013, 563, 1-8.	2.6	32
40	Experimental inelastic neutron scattering spectrum of hydrogen hexagonal clathrate-hydrate compared with rigorous quantum simulations. Journal of Chemical Physics, 2013, 139, 164507.	3.0	20
41	Quantum calculation of inelastic neutron scattering spectra of a hydrogen molecule inside a nanoscale cavity based on rigorous treatment of the coupled translation-rotation dynamics. Physical Review B, 2011, 83, .	3.2	52
42	Theory and spectroscopy of an incarcerated quantum rotor: The infrared spectroscopy, inelastic neutron scattering and nuclear magnetic resonance of H2@C60 at cryogenic temperature. Coordination Chemistry Reviews, 2011, 255, 938-948.	18.8	58
43	Inelastic neutron scattering spectra of a hydrogen molecule in a nanocavity: Methodology for quantum calculations incorporating the coupled five-dimensional translation-rotation eigenstates. Physical Review B, 2011, 84, .	3.2	38
44	Path Integral Molecular Dynamics Study of Small H₂ Clusters in the Large Cage of Structure II Clathrate Hydrate: Temperature Dependence of Quantum Spatial Distributions. Journal of Physical Chemistry C, 2010, 114, 20775-20782.	3.1	48
45	Hydrogen Molecules inside Fullerene C₇₀: Quantum Dynamics, Energetics, Maximum Occupancy, And Comparison with C₆₀. Journal of the American Chemical Society, 2010, 132, 9826-9832.	13.7	51
46	Quantum Dynamics of a Hydrogen Molecule Inside an Anisotropic Open-Cage Fullerene: Coupled Translation-Rotation Eigenstates and Comparison with Inelastic Neutron Scattering Spectroscopy. Journal of Physical Chemistry A, 2010, 114, 9936-9947.	2.5	17
47	Quantum Dynamics of the Vibrations of Helium Bound to the Nanosurface of a Large Planar Organic Molecule: PhthalocyanineÂ·He van der Waals Complex. Journal of Physical Chemistry A, 2009, 113, 3789-3798.	2.5	4
48	Coupled translation-rotation eigenstates of H2 in C60 and C70 on the spectroscopically optimized interaction potential: Effects of cage anisotropy on the energy level structure and assignments. Journal of Chemical Physics, 2009, 130, 224306.	3.0	69
49	Methane molecule confined in the small and large cages of structure I clathrate hydrate: Quantum six-dimensional calculations of the coupled translation-rotation eigenstates. Journal of Chemical Physics, 2009, 131, 224308.	3.0	20
50	Coupled Translationâ^'Rotation Eigenstates of H₂, HD, and D₂ in the Large Cage of Structure II Clathrate Hydrate: Comparison with the Small Cage and Rotational Raman Spectroscopy. Journal of Physical Chemistry A, 2009, 113, 7601-7609.	2.5	41
51	Quantum dynamics of coupled translational and rotational motions of H2 inside C60. Journal of Chemical Physics, 2008, 128, 011101.	3.0	74
52	Quantum dynamics of small H2 and D2 clusters in the large cage of structure II clathrate hydrate: Energetics, occupancy, and vibrationally averaged cluster structures. Journal of Chemical Physics, 2008, 129, 244706.	3.0	59
53	Quantum dynamics of H2, D2, and HD in the small dodecahedral cage of clathrate hydrate: Evaluating H2-water nanocage interaction potentials by comparison of theory with inelastic neutron scattering experiments. Journal of Chemical Physics, 2008, 128, 244715.	3.0	66
54	H 2 , HD, and D2 inside C60: Coupled translation-rotation eigenstates of the endohedral molecules from quantum five-dimensional calculations. Journal of Chemical Physics, 2008, 129, 064313.	3.0	80

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55	One and Two Hydrogen Molecules in the Large Cage of the Structure II Clathrate Hydrate:â€‰ Quantum Translationâ^'Rotation Dynamics Close to the Cage Wall. Journal of Physical Chemistry A, 2007, 111, 6115-6121.	2.5	27
56	Hydrogen Molecules in the Small Dodecahedral Cage of a Clathrate Hydrate:â€‰ Quantum Translationâ^'Rotation Dynamics of the Confined Molecules. Journal of Physical Chemistry C, 2007, 111, 2497-2504.	3.1	45
57	Wave Function Delocalization and Large-Amplitude Vibrations of Helium on Corrugated Aromatic Microsurfaces:Â TetraceneÂ·He and PentaceneÂ·He van der Waals Complexesâ€. Journal of Physical Chemistry A, 2007, 111, 7653-7663.	2.5	5
58	Hydrogen Molecule in the Small Dodecahedral Cage of a Clathrate Hydrate:â€‰ Quantum Translationâ^'Rotation Dynamics at Higher Excitation Energies. Journal of Physical Chemistry A, 2007, 111, 12763-12771.	2.5	30
59	Hydrogen Molecule in the Small Dodecahedral Cage of a Clathrate Hydrate:Â Quantum Five-Dimensional Calculations of the Coupled Translationâ^'Rotation Eigenstates. Journal of Physical Chemistry B, 2006, 110, 24806-24811.	2.6	83
60	HF in clusters of molecular hydrogen: II. Quantum solvation by H2 isotopomers, cluster rigidity, and comparison with CO-doped parahydrogen clusters. Journal of Chemical Physics, 2006, 125, 164313.	3.0	10
61	HF in clusters of molecular hydrogen. I. Size evolution of quantum solvation by parahydrogen molecules. Journal of Chemical Physics, 2005, 122, 244306.	3.0	13
62	(HCl)2 and (HF)2 in small helium clusters: Quantum solvation of hydrogen-bonded dimers. Journal of Chemical Physics, 2005, 123, 224313.	3.0	17
63	Ar[sub n]HF van der Waals clusters revisited. I. New low-energy isomeric structures for n=6â€“13. Journal of Chemical Physics, 2004, 121, 11045.	3.0	6
64	Intermolecular potential energy surface and spectra of Heâ€“HCl with generalization to other rare gasâ€“hydrogen halide complexes. Journal of Chemical Physics, 2004, 121, 11839-11855.	3.0	37
65	A theoretical study of vibrational mode coupling in H5O2+. Journal of Chemical Physics, 2003, 119, 6571-6580.	3.0	79
66	Clusters containing open-shell molecules. III. Quantum five-dimensional/two-surface bound-state calculations on ArnOH van der Waals clusters (X2Î, n=4 to 12). Journal of Chemical Physics, 2002, 117, 4787-4799.	3.0	6
67	Clusters containing open-shell molecules. II. Equilibrium structures of ArnOH Van der Waals clusters (X2Î, n=1 to 15). Journal of Chemical Physics, 2002, 117, 4777-4786.	3.0	11
68	HF Dimer in Small Helium Clusters: Interchange-Tunneling Dynamics in a Quantum Environment. Physical Review Letters, 2002, 88, 123401.	7.8	22
69	Reduced-dimensionality quantum bound state treatment of hydrogen-bonded clusters: torsional vibrational manifold of the water trimer. Computer Physics Communications, 2002, 145, 184-193.	7.5	2
70	Relative stabilities of the two isomers of the methanol-water dimer: The effects of the internal rotations of the hydroxyl and methyl groups of methanol. Journal of Chemical Physics, 2001, 114, 10294-10299.	3.0	14
71	Fully coupled six-dimensional calculations of rovibrational eigenstates of floppy four-atom molecules. Computer Physics Communications, 2000, 128, 46-54.	7.5	8
72	Calculated and experimental rotational constants of (H2O)3: Effects of intermolecular torsional and symmetric stretching excitations. Journal of Chemical Physics, 1999, 111, 10727-10729.	3.0	15

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73	Six-dimensional quantum treatment of the vibrations of diatomic adsorbates on solid surfaces: CO on Cu(100). Journal of Chemical Physics, 1999, 111, 11164-11176.	3.0	40
74	Nonadditive intermolecular forces in Arnâ€“HF van der Waals clusters: Effects on the HF vibrational frequency shift. Journal of Chemical Physics, 1999, 111, 8378-8383.	3.0	31
75	Calculated and experimental rotational constants of (D2O)3: Effects of intermolecular torsional and symmetric stretching excitations. Journal of Chemical Physics, 1999, 111, 5331-5337.	3.0	17
76	Rotational constants of all H/D substituted water trimers: Coupling of intermolecular torsional and symmetric stretching modes. Journal of Chemical Physics, 1999, 110, 5745-5757.	3.0	25
77	Six-dimensional quantum calculations of vibration-rotation-tunneling levels of Î½1 and Î½2 HCl-stretching excited (HCl)2. Journal of Chemical Physics, 1998, 108, 4804-4816.	3.0	66
78	Four-dimensional model calculation of torsional levels of cyclic water tetramer. Journal of Chemical Physics, 1998, 109, 5404-5419.	3.0	28
79	Vibration-rotation-tunneling dynamics of (HF)2 and (HCl)2 from full-dimensional quantum bound-state calculations. Advances in Molecular Vibrations and Collision Dynamics, 1998, , 183-204.	0.8	4
80	Exact six-dimensional quantum calculations of the rovibrational levels of (HCl)2. Journal of Chemical Physics, 1997, 106, 2158-2170.	3.0	63
81	Very large amplitude intermolecular vibrations and wave function delocalization in 2,3-dimethylnaphthaleneâ‹…He van der Waals complex. Journal of Chemical Physics, 1997, 107, 8781-8793.	3.0	26
82	Size and isomer dependence of HF vibrational frequency shift in ArnHF van der Waals clusters with n=1â€“14. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 1459-1466.	1.7	16
83	Three-dimensional model treatment of the torsional levels of isotopic water trimers. Chemical Physics Letters, 1996, 261, 318-328.	2.6	35
84	ArnHF (n = 1â€“4) van der Waals clusters: a quantum Monte Carlo study of ground state energies, structures and HF vibrational frequency shifts. Chemical Physics Letters, 1996, 252, 23-32.	2.6	49
85	Resonances in the UV photodissociation of the Arâ€¦HCl van der Waals complex? An exact quantum 3D wave packet study. Chemical Physics Letters, 1995, 235, 316-320.	2.6	28
86	Three-dimensional model calculation of torsional levels of (H2O)3 and (D2O)3. Chemical Physics Letters, 1995, 244, 283-294.	2.6	67
87	Spectroscopy and quantum dynamics of the 1,2â€dimethylnaphthaleneâ‹…Ar van der Waals complex. Journal of Chemical Physics, 1995, 102, 4715-4725.	3.0	9
88	Exact fullâ€dimensional bound state calculations for (HF)2, (DF)2, and HFDF. Journal of Chemical Physics, 1995, 102, 2315-2325.	3.0	132
89	van der Waals vibrations and isomers of 2,3â€dimethylnaphthaleneâ‹…Ne: Experiment and quantum threeâ€dimensional calculations. Journal of Chemical Physics, 1995, 103, 4855-4868.	3.0	18
90	Isomer dependence of HF vibrational frequency shift for ArnHF (n=4â€“14) van der Waals clusters: Quantum fiveâ€dimensional bound state calculations. Journal of Chemical Physics, 1995, 103, 1829-1841.	3.0	59

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91	Vibrational predissociation of HF dimer in Î½HF=1: Influence of initially excited intermolecular vibrations on the fragmentation dynamics. Journal of Chemical Physics, 1995, 102, 4382-4389.	3.0	25
92	15. Bound States of Strongly Coupled Multidimensional Molecular Hamiltonians by the Discrete Variable Representation Approach. , 1995, , 263-277.		7
93	Resonances in the photodissociation of HCl in the Arâ€“HCl van der Waals complex: How prominent are they?. Journal of Chemical Physics, 1994, 100, 7239-7249.	3.0	52
94	ArnH2O (n=1â€“14) van der Waals clusters: Size evolution of equilibrium structures. Journal of Chemical Physics, 1994, 101, 8310-8320.	3.0	17
95	Quantum threeâ€dimensional calculation of endohedral vibrational levels of atoms inside strongly nonspherical fullerenes: Ne@C70. Journal of Chemical Physics, 1994, 101, 2126-2140.	3.0	17
96	Equilibrium structures and approximate HF vibrational red shifts for ArnHF (n=1â€“14) van der Waals clusters. Journal of Chemical Physics, 1994, 100, 7166-7181.	3.0	67
97	Intermolecular vibrations of the 2,3â€dimethylnaphthaleneâ‹…Ar van der Waals complex: Experiment and quantum threeâ€dimensional calculations. Journal of Chemical Physics, 1994, 100, 52-62.	3.0	30
98	Three-dimensional discrete variable representation for accurate Van der Waals vibrational states of complexes between atoms and large molecules, including fullerenes. Faraday Discussions, 1994, 97, 265-283.	3.2	5
99	HF vibrational redshift for the icosahedral Ar12HF van der Waals cluster is the same as in an Ar matrix: Quantum fiveâ€dimensional bound state calculations. Journal of Chemical Physics, 1994, 101, 6359-6361.	3.0	40
100	Intermolecular vibrations of oâ€xyleneâ‹…Ar in the S0 and S1 states: Experiment and quantum three dimensional calculations. Journal of Chemical Physics, 1994, 101, 6412-6423.	3.0	29
101	van der Waals vibrational states of atomâ€“large molecule complexes by a 3D discrete variable representation method: Naphthaleneâ‹…Ar. Journal of Chemical Physics, 1993, 98, 7165-7178.	3.0	67
102	A timeâ€dependent golden rule wave packet calculation for vibrational predissociation of D2HF. Journal of Chemical Physics, 1992, 97, 927-934.	3.0	40
103	Mode-specific decay widths in vibrational predissociation of D2HF. Chemical Physics Letters, 1992, 194, 313-317.	2.6	15
104	Complex coordinate rotation calculation of branching ratios. International Journal of Quantum Chemistry, 1982, 21, 727-739.	2.0	32
105	Intra- and intermolecular rovibrational states of HCl-H2O and DCl-H2O dimers from full-dimensional and fully coupled quantum calculations. Chinese Journal of Chemical Physics, 0, , .	1.3	9