

Zlatko Bašić

List of Publications by Year in descending order

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105
papers

3,015
citations

136950

32
h-index

206112

48
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106
all docs

106
docs citations

106
times ranked

1096
citing authors

#	ARTICLE	IF	CITATIONS
1	Exact full-dimensional bound state calculations for (HF) ₂ , (DF) ₂ , and HFDF. Journal of Chemical Physics, 1995, 102, 2315-2325.	3.0	132
2	Hydrogen Molecule in the Small Dodecahedral Cage of a Clathrate Hydrate: Quantum Five-Dimensional Calculations of the Coupled Translation-Rotation Eigenstates. Journal of Physical Chemistry B, 2006, 110, 24806-24811.	2.6	83
3	H ₂ , HD, and D ₂ inside C ₆₀ : Coupled translation-rotation eigenstates of the endohedral molecules from quantum five-dimensional calculations. Journal of Chemical Physics, 2008, 129, 064313.	3.0	80
4	A theoretical study of vibrational mode coupling in H ₅ O ₂ ⁺ . Journal of Chemical Physics, 2003, 119, 6571-6580.	3.0	79
5	Quantum dynamics of coupled translational and rotational motions of H ₂ inside C ₆₀ . Journal of Chemical Physics, 2008, 128, 011101.	3.0	74
6	Coupled translation-rotation eigenstates of H ₂ in C ₆₀ and C ₇₀ 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
7	van der Waals vibrational states of atom-large molecule complexes by a 3D discrete variable representation method: Naphthalene...Ar. Journal of Chemical Physics, 1993, 98, 7165-7178.	3.0	67
8	Equilibrium structures and approximate HF vibrational red shifts for Ar _n HF (n=1-14) van der Waals clusters. Journal of Chemical Physics, 1994, 100, 7166-7181.	3.0	67
9	Three-dimensional model calculation of torsional levels of (H ₂ O) ₃ and (D ₂ O) ₃ . Chemical Physics Letters, 1995, 244, 283-294.	2.6	67
10	Six-dimensional quantum calculations of vibration-rotation-tunneling levels of $\hat{v}_{1/2}^1$ and $\hat{v}_{1/2}^2$ HCl-stretching excited (HCl) ₂ . Journal of Chemical Physics, 1998, 108, 4804-4816.	3.0	66
11	Quantum dynamics of H ₂ , D ₂ , and HD in the small dodecahedral cage of clathrate hydrate: Evaluating H ₂ -water nanocage interaction potentials by comparison of theory with inelastic neutron scattering experiments. Journal of Chemical Physics, 2008, 128, 244715.	3.0	66
12	Exact six-dimensional quantum calculations of the rovibrational levels of (HCl) ₂ . Journal of Chemical Physics, 1997, 106, 2158-2170.	3.0	63
13	Isomer dependence of HF vibrational frequency shift for Ar _n HF (n=4-14) van der Waals clusters: Quantum five-dimensional bound state calculations. Journal of Chemical Physics, 1995, 103, 1829-1841.	3.0	59
14	Quantum dynamics of small H ₂ and D ₂ 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
15	Theory and spectroscopy of an incarcerated quantum rotor: The infrared spectroscopy, inelastic neutron scattering and nuclear magnetic resonance of H ₂ @C ₆₀ at cryogenic temperature. Coordination Chemistry Reviews, 2011, 255, 938-948.	18.8	58
16	Resonances in the photodissociation of HCl in the Ar-HCl van der Waals complex: How prominent are they?. Journal of Chemical Physics, 1994, 100, 7239-7249.	3.0	52
17	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
18	Hydrogen Molecules inside Fullerene C ₇₀ : Quantum Dynamics, Energetics, Maximum Occupancy, And Comparison with C ₆₀ . Journal of the American Chemical Society, 2010, 132, 9826-9832.	13.7	51

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19	Ar _n HF (n = 1–4) van der Waals clusters: a quantum Monte Carlo study of ground state energies, structures and HF vibrational frequency shifts. <i>Chemical Physics Letters</i> , 1996, 252, 23-32.	2.6	49
20	Path Integral Molecular Dynamics Study of Small H ₂ Clusters in the Large Cage of Structure II Clathrate Hydrate: Temperature Dependence of Quantum Spatial Distributions. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20775-20782.	3.1	48
21	Hydrogen Molecules in the Small Dodecahedral Cage of a Clathrate Hydrate: Quantum Translation-Rotation Dynamics of the Confined Molecules. <i>Journal of Physical Chemistry C</i> , 2007, 111, 2497-2504.	3.1	45
22	Coupled Translation-Rotation Eigenstates of H ₂ , HD, and D ₂ in the Large Cage of Structure II Clathrate Hydrate: Comparison with the Small Cage and Rotational Raman Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7601-7609.	2.5	41
23	A time-dependent golden rule wave packet calculation for vibrational predissociation of D ₂ HF. <i>Journal of Chemical Physics</i> , 1992, 97, 927-934.	3.0	40
24	HF vibrational redshift for the icosahedral Ar ₁₂ HF van der Waals cluster is the same as in an Ar matrix: Quantum five-dimensional bound state calculations. <i>Journal of Chemical Physics</i> , 1994, 101, 6359-6361.	3.0	40
25	Six-dimensional quantum treatment of the vibrations of diatomic adsorbates on solid surfaces: CO on Cu(100). <i>Journal of Chemical Physics</i> , 1999, 111, 11164-11176.	3.0	40
26	Efficient Calculation of Free Energy Differences Associated with Isotopic Substitution Using Path-Integral Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1440-1453.	5.3	39
27	Inelastic neutron scattering spectra of a hydrogen molecule in a nanocavity: Methodology for quantum calculations incorporating the coupled five-dimensional translation-rotation eigenstates. <i>Physical Review B</i> , 2011, 84, .	3.2	38
28	Intermolecular potential energy surface and spectra of He-HCl with generalization to other rare gas-hydrogen halide complexes. <i>Journal of Chemical Physics</i> , 2004, 121, 11839-11855.	3.0	37
29	Communication: Quantum six-dimensional calculations of the coupled translation-rotation eigenstates of H ₂ O@C ₆₀ . <i>Journal of Chemical Physics</i> , 2016, 144, 201101.	3.0	36
30	Explaining the symmetry breaking observed in the endofullerenes H ₂ @C ₆₀ , HF@C ₆₀ , and H ₂ O@C ₆₀ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31274-31283.	2.8	36
31	Three-dimensional model treatment of the torsional levels of isotopic water trimers. <i>Chemical Physics Letters</i> , 1996, 261, 318-328.	2.6	35
32	Neutron Scattering Measurements and Computation of the Quantum Dynamics of Hydrogen Molecules Trapped in the Small and Large Cages of Clathrate Hydrates. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7314-7326.	2.5	33
33	Complex coordinate rotation calculation of branching ratios. <i>International Journal of Quantum Chemistry</i> , 1982, 21, 727-739.	2.0	32
34	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. <i>Chemical Physics Letters</i> , 2013, 563, 1-8.	2.6	32
35	Nonadditive intermolecular forces in Ar _n HF van der Waals clusters: Effects on the HF vibrational frequency shift. <i>Journal of Chemical Physics</i> , 1999, 111, 8378-8383.	3.0	31
36	Competing quantum effects in the free energy profiles and diffusion rates of hydrogen and deuterium molecules through clathrate hydrates. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32169-32177.	2.8	31

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37	Intermolecular vibrations of the 2,3-dimethylnaphthalene...Ar van der Waals complex: Experiment and quantum three-dimensional calculations. Journal of Chemical Physics, 1994, 100, 52-62.	3.0	30
38	Hydrogen Molecule in the Small Dodecahedral Cage of a Clathrate Hydrate: Quantum Translation-Rotation Dynamics at Higher Excitation Energies. Journal of Physical Chemistry A, 2007, 111, 12763-12771.	2.5	30
39	Intermolecular vibrations of o-xylene...Ar in the S0 and S1 states: Experiment and quantum three dimensional calculations. Journal of Chemical Physics, 1994, 101, 6412-6423.	3.0	29
40	Inelastic neutron scattering spectrum of H ₂ @C ₆₀ and its temperature dependence decoded using rigorous quantum calculations and a new selection rule. Journal of Chemical Physics, 2013, 139, 064309.	3.0	29
41	Resonances in the UV photodissociation of the Ar HCl van der Waals complex? An exact quantum 3D wave packet study. Chemical Physics Letters, 1995, 235, 316-320.	2.6	28
42	Four-dimensional model calculation of torsional levels of cyclic water tetramer. Journal of Chemical Physics, 1998, 109, 5404-5419.	3.0	28
43	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
44	HCl-H ₂ O 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
45	One and Two Hydrogen Molecules in the Large Cage of the Structure II Clathrate Hydrate: Quantum Translation-Rotation Dynamics Close to the Cage Wall. Journal of Physical Chemistry A, 2007, 111, 6011-6019. Confirming a Predicted Selection Rule in Inelastic Neutron Scattering Spectroscopy: The Quantum Translator-Rotator	2.5	27
46	Very large amplitude intermolecular vibrations and wave function delocalization in H ₂ entrapped inside C ₆₀	7.8	27
47	Very large amplitude intermolecular vibrations and wave function delocalization in 2,3-dimethylnaphthalene...He van der Waals complex. Journal of Chemical Physics, 1997, 107, 8781-8793.	3.0	26
48	Vibrational predissociation of HF dimer in $\hat{1}/2$ HF=1: Influence of initially excited intermolecular vibrations on the fragmentation dynamics. Journal of Chemical Physics, 1995, 102, 4382-4389.	3.0	25
49	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
50	H ₂ , HD, and D ₂ 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
51	Flexible water molecule in C ₆₀ : 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
52	Intramolecular stretching vibrational states and frequency shifts of (H ₂) 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
53	HF Dimer in Small Helium Clusters: Interchange-Tunneling Dynamics in a Quantum Environment. Physical Review Letters, 2002, 88, 123401.	7.8	22
54	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

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55	Electric-dipole-coupled $H_2O@C_{60}$ dimer: Translation-rotation eigenstates from twelve-dimensional quantum calculations. <i>Journal of Chemical Physics</i> , 2017, 146, 084303.	3.0	22
56	Perspective: Accurate treatment of the quantum dynamics of light molecules inside fullerene cages: Translation-rotation states, spectroscopy, and symmetry breaking. <i>Journal of Chemical Physics</i> , 2018, 149, 100901.	3.0	22
57	$H_2O@CO$ and $D_2O@CO$ complexes: Intra- and intermolecular rovibrational states from full-dimensional and fully coupled quantum calculations. <i>Journal of Chemical Physics</i> , 2020, 153, 074107.	3.0	21
58	Methane molecule confined in the small and large cages of structure I clathrate hydrate: Quantum six-dimensional calculations of the coupled translation-rotation eigenstates. <i>Journal of Chemical Physics</i> , 2009, 131, 224308.	3.0	20
59	Experimental inelastic neutron scattering spectrum of hydrogen hexagonal clathrate-hydrate compared with rigorous quantum simulations. <i>Journal of Chemical Physics</i> , 2013, 139, 164507.	3.0	20
60	General Selection Rule in the Inelastic Neutron Scattering Spectroscopy of a Diatomic Molecule Confined Inside a Near-Spherical Nanocavity. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3721-3725.	4.6	20
61	Effects of symmetry breaking on the translation-rotation eigenstates of H_2 , HF, and H_2O inside the fullerene C_{60} . <i>Faraday Discussions</i> , 2018, 212, 547-567.	3.2	20
62	The von Neumann basis in non-Cartesian coordinates: Application to floppy triatomic molecules. <i>Journal of Chemical Physics</i> , 2014, 141, 234106.	3.0	19
63	van der Waals vibrations and isomers of 2,3-dimethylnaphthalene...Ne: Experiment and quantum three-dimensional calculations. <i>Journal of Chemical Physics</i> , 1995, 103, 4855-4868.	3.0	18
64	Impact of the Condensed-Phase Environment on the Translation-Rotation Eigenstates and Spectra of a Hydrogen Molecule in Clathrate Hydrates. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 308-313.	4.6	18
65	Ar_nH_2O ($n=1-14$) van der Waals clusters: Size evolution of equilibrium structures. <i>Journal of Chemical Physics</i> , 1994, 101, 8310-8320.	3.0	17
66	Quantum three-dimensional calculation of endohedral vibrational levels of atoms inside strongly nonspherical fullerenes: $Ne@C_{70}$. <i>Journal of Chemical Physics</i> , 1994, 101, 2126-2140.	3.0	17
67	Calculated and experimental rotational constants of $(D_2O)_3$: Effects of intermolecular torsional and symmetric stretching excitations. <i>Journal of Chemical Physics</i> , 1999, 111, 5331-5337.	3.0	17
68	$(HCl)_2$ and $(HF)_2$ in small helium clusters: Quantum solvation of hydrogen-bonded dimers. <i>Journal of Chemical Physics</i> , 2005, 123, 224313.	3.0	17
69	Quantum Dynamics of a Hydrogen Molecule Inside an Anisotropic Open-Cage Fullerene: Coupled Translation-Rotation Eigenstates and Comparison with Inelastic Neutron Scattering Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9936-9947.	2.5	17
70	Size and isomer dependence of HF vibrational frequency shift in Ar_nHF van der Waals clusters with $n=1-14$. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 1459-1466.	1.7	16
71	The HD molecule in small and medium cages of clathrate hydrates: Quantum dynamics studied by neutron scattering measurements and computation. <i>Journal of Chemical Physics</i> , 2014, 141, 134501.	3.0	16
72	The effect of the condensed-phase environment on the vibrational frequency shift of a hydrogen molecule inside clathrate hydrates. <i>Journal of Chemical Physics</i> , 2018, 148, 144304.	3.0	16

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73	Mode-specific decay widths in vibrational predissociation of D ₂ HF. <i>Chemical Physics Letters</i> , 1992, 194, 313-317.	2.6	15
74	Calculated and experimental rotational constants of (H ₂ O) ₃ : Effects of intermolecular torsional and symmetric stretching excitations. <i>Journal of Chemical Physics</i> , 1999, 111, 10727-10729.	3.0	15
75	Translation-rotation states of H ₂ in C ₆₀ : New insights from a perturbation-theory treatment. <i>Journal of Chemical Physics</i> , 2016, 145, 084310.	3.0	15
76	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. <i>Journal of Chemical Physics</i> , 2001, 114, 10294-10299.	3.0	14
77	HDO- ¹³ C ¹⁸ O Complex: D-Bonded and H-Bonded Isomers and Intra- and Intermolecular Rovibrational States from Full-Dimensional and Fully Coupled Quantum Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 980-989.	2.5	14
78	HF in clusters of molecular hydrogen. I. Size evolution of quantum solvation by parahydrogen molecules. <i>Journal of Chemical Physics</i> , 2005, 122, 244306.	3.0	13
79	Benzene- ¹⁸ O ₂ and benzene- ¹⁸ O ¹⁷ O: Fully coupled nine-dimensional quantum calculations of flexible H ₂ O/HDO intramolecular vibrational excitations and intermolecular states of the dimers, and their infrared and Raman spectra using compact bases. <i>Journal of Chemical Physics</i> , 2020, 152, 124103.	3.0	13
80	Enhanced Sampling Path Integral Methods Using Neural Network Potential Energy Surfaces with Application to Diffusion in Hydrogen Hydrates. <i>Advanced Theory and Simulations</i> , 2021, 4, 2000258.	2.8	13
81	Clusters containing open-shell molecules. II. Equilibrium structures of ArOH Van der Waals clusters (X ² , n=1 to 15). <i>Journal of Chemical Physics</i> , 2002, 117, 4777-4786.	3.0	11
82	The Endofullerene HF@C ₆₀ : Inelastic Neutron Scattering Spectra from Quantum Simulations and Experiment, Validity of the Selection Rule, and Symmetry Breaking. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5365-5371.	4.6	11
83	DCl- ¹⁸ O ₂ , HCl- ¹⁸ O ₂ , and DCl- ¹⁸ O ₂ Dimers: Inter- and Intramolecular Vibrational States and Frequency Shifts from Fully Coupled Quantum Calculations on a Full-Dimensional Neural Network Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6437-6449.	2.5	11
84	HF in clusters of molecular hydrogen: II. Quantum solvation by H ₂ isotopomers, cluster rigidity, and comparison with CO-doped parahydrogen clusters. <i>Journal of Chemical Physics</i> , 2006, 125, 164313.	3.0	10
85	Accurate quantum calculations of translation-rotation eigenstates in electric-dipole-coupled H ₂ O@C ₆₀ assemblies. <i>Chemical Physics Letters</i> , 2017, 683, 172-178.	2.6	10
86	An open-chain imaginary-time path-integral sampling approach to the calculation of approximate symmetrized quantum time correlation functions. <i>Journal of Chemical Physics</i> , 2018, 148, 102340.	3.0	10
87	Light molecules inside the nanocavities of fullerenes and clathrate hydrates: inelastic neutron scattering spectra and the unexpected selection rule from rigorous quantum simulations. <i>International Reviews in Physical Chemistry</i> , 2020, 39, 425-463.	2.3	10
88	Spectroscopy and quantum dynamics of the 1,2-dimethylnaphthalene...Ar van der Waals complex. <i>Journal of Chemical Physics</i> , 1995, 102, 4715-4725.	3.0	9
89	Intra- and intermolecular rovibrational states of HCl-H ₂ O and DCl-H ₂ O dimers from full-dimensional and fully coupled quantum calculations. <i>Chinese Journal of Chemical Physics</i> , 0, , .	1.3	9
90	Fully coupled six-dimensional calculations of rovibrational eigenstates of floppy four-atom molecules. <i>Computer Physics Communications</i> , 2000, 128, 46-54.	7.5	8

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91	15. Bound States of Strongly Coupled Multidimensional Molecular Hamiltonians by the Discrete Variable Representation Approach. , 1995, , 263-277.		7
92	H ₂ 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
93	Clusters containing open-shell molecules. III. Quantum five-dimensional/two-surface bound-state calculations on ArOH van der Waals clusters (X ² 1, n=4 to 12). Journal of Chemical Physics, 2002, 117, 4787-4799.	3.0	6
94	Ar _[sub n] HF van der Waals clusters revisited. I. New low-energy isomeric structures for n=6-13. Journal of Chemical Physics, 2004, 121, 11045.	3.0	6
95	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
96	Wave Function Delocalization and Large-Amplitude Vibrations of Helium on Corrugated Aromatic Microsurfaces: Tetracene-He and Pentacene-He van der Waals Complexes. Journal of Physical Chemistry A, 2007, 111, 7653-7663.	2.5	5
97	Intermolecular rovibrational states of the H ₂ O-CO ₂ and D ₂ O-CO ₂ van der Waals complexes. Journal of Chemical Physics, 2022, 156, 064301.	3.0	5
98	Quantum Dynamics of the Vibrations of Helium Bound to the Nanosurface of a Large Planar Organic Molecule: Phthalocyanine-He van der Waals Complex. Journal of Physical Chemistry A, 2009, 113, 3789-3798.	2.5	4
99	Molecules in confinement in clusters, quantum solvents and matrices: general discussion. Faraday Discussions, 2018, 212, 569-601.	3.2	4
100	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
101	H ₂ O inside the fullerene C ₆₀ : Inelastic neutron scattering spectrum from rigorous quantum calculations. Journal of Chemical Physics, 2022, 156, 124101.	3.0	3
102	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
103	Precise characterisation of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 137-155.	3.2	1
104	Hydrogen Intramolecular Stretch Redshift in the Electrostatic Environment of Type II Clathrate Hydrates from Schrödinger Equation Treatment. Applied Sciences (Switzerland), 2020, 10, 8504.	2.5	1
105	Tribute to Joel M. Bowman. Journal of Physical Chemistry A, 2013, 117, 6905-6906.	2.5	0