Rita Prosmiti

List of Publications by Year
in descending order

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Version: 2024-02-01

64 papers	1,129 citations	331670 21 h-index	454955 30 g-index
64 all docs	64 docs citations	64 times ranked	468 citing authors

#	Article	IF	Citations
1	Assessment of DFT approaches in noble gas clathrate-like clusters: stability and thermodynamics. Physical Chemistry Chemical Physics, 2022, 24, 1475-1485.	2.8	8
2	Unraveling the Origin of Symmetry Breaking in H₂O@C₆₀ Endofullerene Through Quantum Computations. ChemPhysChem, 2022, 23, e202200034.	2.1	6
3	A Benchmark Protocol for DFT Approaches and Data-Driven Models for Halide-Water Clusters. Molecules, 2022, 27, 1654.	3.8	5
4	Delving into guest-free and He-filled sI and sII clathrate hydrates: a first-principles computational study. Physical Chemistry Chemical Physics, 2022, 24, 13119-13129.	2.8	4
5	Quantum molecular simulations of micro-hydrated halogen anions. Physical Chemistry Chemical Physics, 2022, 24, 14964-14974.	2.8	2
6	Modelling interactions of cationic dimers in He droplets: microsolvation trends in He_nK₂⁺ clusters. Physical Chemistry Chemical Physics, 2021, 23, 7849-7859.	2.8	7
7	Exploring CO₂@sI Clathrate Hydrates as CO₂ Storage Agents by Computational Density Functional Approaches. ChemPhysChem, 2021, 22, 359-369.	2.1	11
8	Encapsulation of a Water Molecule inside C₆₀ Fullerene: The Impact of Confinement on Quantum Features. Journal of Chemical Theory and Computation, 2021, 17, 5839-5848.	5.3	16
9	Computational density-functional approaches on finite-size and guest-lattice effects in CO2@sII clathrate hydrate. Journal of Chemical Physics, 2021, 154, 044301.	3.0	10
10	Structural Stability of the CO₂@sI Hydrate: a Bottomâ€Up Quantum Chemistry Approach on the Guestâ€Cage and Interâ€Cage Interactions. ChemPhysChem, 2020, 21, 2618-2628.	2.1	9
11	He Inclusion in Ice-like and Clathrate-like Frameworks: A Benchmark Quantum Chemistry Study of Guestâ€“Host Interactions. Journal of Chemical Information and Modeling, 2020, 60, 3043-3056.	5.4	13
12	Finite Systems under Pressure: Assessing Volume Definition Models from Parallel-Tempering Monte Carlo Simulations. Journal of Physical Chemistry A, 2020, 124, 4036-4047.	2.5	6
13	The smallest proton-bound dimer H ₅ ⁺ : theoretical progress. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180396.	3.4	1
14	Theoretical Study of Cationic Alkali Dimers Interacting with He: Li₂⁺â€“He and Na₂⁺â€“He van der Waals Complexes. Journal of Physical Chemistry A, 2019, 123, 7814-7821.	2.5	9
15	Quantum effects on the stability of the He₅I₂ van der Waals conformers. Journal of Computational Chemistry, 2019, 40, 2200-2206.	3.3	0
16	Assessing Intermolecular Interactions in Guest-Free Clathrate Hydrate Systems. Journal of Physical Chemistry A, 2018, 122, 1479-1487.	2.5	15
17	Fully Coupled Quantum Treatment of Nanoconfined Systems: A Water Molecule inside a Fullerene C60. Journal of Chemical Theory and Computation, 2018, 14, 6521-6531.	5.3	13
18	A Systematic Protocol for Benchmarking Guestâ€“Host Interactions by Firstâ€Principles Computations: Capturing CO₂ in Clathrate Hydrates. Chemistry - A European Journal, 2018, 24, 9353-9363.	3.3	13

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19	Preferential stabilization of HeI2 van der Waals isomers: the effect of energetics and temperature. RSC Advances, 2017, 7, 19273-19279.	3.6	4
20	Developing time to frequency-domain descriptors for relaxation processes: Local trends. Journal of Molecular Liquids, 2017, 245, 62-70.	4.9	1
21	High Pressure Structural Transitions in Kr Clathrate-Like Clusters. Journal of Physical Chemistry C, 2016, 120, 26093-26102.	3.1	14
22	Temperature Dependence of HeBr₂ Isomersâ€™ Stability through Rovibrational Multiconfiguration Time-Dependent Hartree Calculations. Journal of Physical Chemistry A, 2016, 120, 9458-9464.	2.5	9
23	i-TTM Model for Ab Initio-Based Ionâ€“Water Interaction Potentials. 1. Halideâ€“Water Potential Energy Functions. Journal of Physical Chemistry B, 2016, 120, 1822-1832.	2.6	61
24	Vibrational Calculations of Higher-Order Weakly Bound Complexes: The He_{3,4}I₂ Cases. Journal of Physical Chemistry A, 2015, 119, 12736-12741.	2.5	2
25	Quantum Features of Anionic Species He^{*â€“} and He₂^{*â€“} in Small He_N Clusters. Journal of Physical Chemistry A, 2015, 119, 11574-11582.	2.5	5
26	Quantum Dynamics of Carbon Dioxide Encapsulated in the Cages of the sI Clathrate Hydrate: Structural Guest Distributions and Cage Occupation. Journal of Physical Chemistry C, 2015, 119, 3945-3956.	3.1	21
27	Thermodynamics of Water Dimer Dissociation in the Primary Hydration Shell of the Iodide Ion with Temperature-Dependent Vibrational Predissociation Spectroscopy. Journal of Physical Chemistry A, 2015, 119, 1859-1866.	2.5	37
28	Reactive scattering calculations for 87Rb+87RbHeâ†'Rb2(3Î£u+,v)+He from ultralow to intermediate energies. Journal of Chemical Physics, 2015, 142, 164304.	3.0	8
29	Theoretical predictions on the role of the internal H3+ rotation in the IR spectra of the H5+ and D5+ cations. Physical Chemistry Chemical Physics, 2014, 16, 6217.	2.8	9
30	Energetics and Solvation Structure of a Dihalogen Dopant (I₂) in ⁴He Clusters. Journal of Physical Chemistry A, 2014, 118, 6492-6500.	2.5	15
31	First-principles simulations of vibrational states and spectra for and clusters using multiconfiguration time-dependent Hartree approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 26-33.	3.9	6
32	Simulating liquid water for determining its structural and transport properties. Applied Radiation and Isotopes, 2014, 83, 115-121.	1.5	4
33	A DFTâ€based potential energy surface for the H cluster. International Journal of Quantum Chemistry, 2013, 113, 651-655.	2.0	8
34	MULTIMODE calculations of the infrared spectra of H 7 + and D 7 + using ab initio potential energy and dipole moment surfaces. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	14
35	Theoretical Investigation of the Infrared Spectra of the H₅⁺ and D₅⁺ Cations. Journal of Physical Chemistry A, 2013, 117, 9518-9524.	2.5	24
36	Quantum Mechanical Characterization of the He₄ICl Weakly Bound Complex. Journal of Physical Chemistry A, 2013, 117, 7217-7223.	2.5	6

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37	Full-dimensional quantum calculations of the dissociation energy, zero-point, and 10 K properties of ${m H}_{7}^{+}$H7+/${m D}_{7}^{+}$D7+ clusters using an ab initio potential energy surface. Journal of Chemical Physics, 2013, 139, 024308.	3.0	9
38	Quantum-dynamics study of the ${m H}_5^+$H5+ cluster: Full dimensional benchmark results on its vibrational states. Journal of Chemical Physics, 2012, 136, 104302.	3.0	26
39	Vibrational dynamics of the ${m H}_5^+$H5+ and its isotopologues from multiconfiguration time-dependent Hartree calculations. Journal of Chemical Physics, 2012, 137, 214308.	3.0	23
40	Full-dimensional (15-dimensional) ab initio analytical potential energy surface for the ${m H}_7^+$H7+ cluster. Journal of Chemical Physics, 2012, 136, 224302.	3.0	15
41	An ab Initio Study of the E ³Î_g State of the Iodine Molecule. Journal of Physical Chemistry A, 2012, 116, 2366-2370.	2.5	14
42	Theoretical investigation of the Heâ€“I2(E3Îg) ion-pair state: Ab initio intermolecular potential and vibrational levels. Journal of Chemical Physics, 2012, 137, 034303.	3.0	19
43	Theoretical simulations of the vibrational predissociation spectra of H 5 + and D 5 + clusters. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	10
44	A theoretical characterization of multiple isomers of the He2I2 complex. Chemical Physics, 2012, 399, 39-45.	1.9	12
45	Internal Proton Transfer and H₂ Rotations in the H₅⁺ Cluster: A Marked Influence on Its Thermal Equilibrium State. Journal of Physical Chemistry A, 2011, 115, 2483-2488.	2.5	30
46	Ab initio characterization of the Neâ€“I2 van der Waals complex: Intermolecular potentials and vibrational bound states. Journal of Chemical Physics, 2011, 134, 214304.	3.0	24
47	Global potential energy surface for the ground electronic state of H: A DFT approach. International Journal of Quantum Chemistry, 2011, 111, 368-374.	2.0	12
48	Infrared spectrum of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub><mml:msup><mml:mrow /><mml:mo>+</mml:mo></mml:msup></mml:mrow></mml:math>and D<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub><mml:msup>	2.5	19
49	Full-dimensional multi configuration time dependent Hartree calculations of the ground and vibrationally excited states of He2,3Br2 clusters. Journal of Chemical Physics, 2011, 135, 054303.	3.0	9
50	Toward a realistic density functional theory potential energy surface for the H5+ cluster. Journal of Chemical Physics, 2010, 133, 054303.	3.0	24
51	Structuring a Quantum Solvent around a Weakly Bound Dopant: The Heâ‹¯Cs₂(³Î£_u) Complex. Journal of Physical Chemistry A, 2009, 113, 14718-14729.	2.5	23
52	Intermolecular Ab Initio Potential and Spectroscopy of the Ground State of HeI₂ Complex Revisited. Journal of Physical Chemistry A, 2009, 113, 5754-5762.	2.5	40
53	Ab initio potential energy surface and spectrum of the B(Î3) state of the HeI2 complex. Journal of Chemical Physics, 2007, 126, 204301.	3.0	31
54	Ab initio vibrational predissociation dynamics of Heâ€“I2(B) complex. Journal of Chemical Physics, 2007, 126, 244314.	3.0	31

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55	A theoretical study of He2ICl van der Waals cluster. Journal of Chemical Physics, 2006, 125, 014313.	3.0	34
56	Ab initio calculations, potential representation and vibrational dynamics of He2Br2 van der Waals complex. Journal of Chemical Physics, 2005, 122, 044305.	3.0	36
57	HeBr2complex: ground-state potential and vibrational dynamics fromab initiocalculations. Molecular Physics, 2004, 102, 2277-2283.	1.7	37
58	Three-Dimensional ab Initio Potential and Ground State Dynamics of the HeI2Complex. Journal of Physical Chemistry A, 2004, 108, 6065-6071.	2.5	36
59	Structures and Energetics of Clusters (n = 5â˜’11). Journal of Physical Chemistry A, 2003, 107, 4768-4772.	2.5	42
60	CCSD(T) intermolecular potential between He atom and ClF molecule: Comparison with experiment. Journal of Chemical Physics, 2003, 119, 4216-4222.	3.0	36
61	He79Br2 B,v=8â†X,vâ€³=0 excitation spectrum: Ab initio prediction and spectroscopic manifestation of a linear isomer. Journal of Chemical Physics, 2002, 117, 6117-6120.	3.0	37
62	The van der Waals potential energy surfaces and structures of Heâ€“ICl and Neâ€“ICl clusters. Journal of Chemical Physics, 2002, 117, 7017-7023.	3.0	51
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