Yu Zhai

List of Publications by Year
in descending order

22	130	1478505 6	1281871 11
papers	citations	h-index	g-index

23	23	23	102
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum vibration perturbation approach with polyatomic probe in simulating infrared spectra. Physical Chemistry Chemical Physics, 2022, 24, 1174-1182.	2.8	2
2	Basis sets dependency in constructing spectroscopy-accuracy Ab Initio global electric dipole moment functions. Chinese Journal of Chemical Physics, 2022, 35, 52-57.	1.3	0
3	Ab initio Morse/long-range potential energy functions plus spectroscopic and thermophysical properties of heteronuclear diatomic complexes of xenon with the rare gases. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 285, 108169.	2.3	7
4	Vibrationally excited intermolecular potential energy surfaces and the predicted near infrared overtone (ν_{OH} = 2 â†•0) spectra of a H₂Oâ€“Ne complex. Physical Chemistry Chemical Physics, 2022, 24, 12937-12949.	2.8	2
5	Ab initio potential energy functions, spectroscopy and thermal physics for krypton-contained rare gas dimers. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 288, 108244.	2.3	3
6	Optical and electrical modulation in ultraviolet photodetectors based on organic oneâ€dimensional photochromic arrays. SmartMat, 2021, 2, 388-397.	10.7	22
7	Outside Back Cover: Volume 2 Issue 3. SmartMat, 2021, 2, ii.	10.7	0
8	A new permutation-symmetry-adapted machine learning diabatization procedure and its application in MgH₂ system. Journal of Chemical Physics, 2021, 155, 214102.	3.0	5
9	Explicitly correlated ab initio potential energy surface and predicted rovibrational spectra for H2Oâ€“N2 and D2Oâ€“N2 complexes. Journal of Chemical Physics, 2020, 153, 054303.	3.0	6
10	Analytic intermolecular potential energy surface and first-principles prediction of the rotational profiles for a symmetric top ion-atom complex: A case study of H3O+â€“Ar. Journal of Chemical Physics, 2020, 152, 214302.	3.0	2
11	Full quantum calculation of the rovibrational states and intensities for a symmetric top-linear molecule dimer: Hamiltonian, basis set, and matrix elements. Journal of Chemical Physics, 2019, 151, 074301.	3.0	6
12	Highly Ordered Semiconducting Polymer Arrays for Sensitive Photodetectors. ACS Applied Materials & Interfaces, 2019, 11, 15829-15836.	8.0	15
13	Theoretical Study of Infrared Spectra of OCS-(pH₂)₂, OCS-(oD₂)₂, OCS-(HD)₂, and Mixed OCS-pH₂-He Trimers. Journal of Physical Chemistry A, 2018, 122, 2915-2926.	2.5	1
14	Constructing high-accuracy intermolecular potential energy surface with multi-dimension Morse/Long-Range model. Molecular Physics, 2018, 116, 843-853.	1.7	11
15	Intermolecular configurations dominated by quadrupoleâ€“quadrupole electrostatic interactions: explicit correlation treatment of the five-dimensional potential energy surface and infrared spectra for the COâ€“N₂ complex. Physical Chemistry Chemical Physics, 2018, 20, 2036-2047.	2.8	15
16	Analytic Morse/long-range potential energy surfaces and â€œadiabatic-hindered-rotorâ€•treatment for a symmetric top-linear molecule dimer: A case study of CH3Fâ€“H2. Journal of Chemical Physics, 2018, 148, 124302.	3.0	10
17	Developments and applications of computational infrared spectroscopy in non-bonded systems: Quantal and classical systems. Chinese Science Bulletin, 2018, 63, 3396-3402.	0.7	1
18	Explicit correlation treatment of the six-dimensional potential energy surface and predicted infrared spectra for OCSâ€“H2. Journal of Chemical Physics, 2017, 147, 044313.	3.0	18

#	Article	IF	Citations
19	The Role of High Excitations in Constructing Sub-spectroscopic Accuracy Intermolecular Potential of He-HCN: Critically Examined by the High-Resolution Spectra with Resonance States. Chinese Journal of Chemical Physics, 2017, 30, 776-788.	1.3	3
20	THE ROLE OF SYMMETRIC-STRETCH VIBRATION IN ASYMMETRIC-STRETCH VIBRATIONAL FREQUENCY SHIFT: THE CASE OF 2CH EXCITATION INFRARED SPECTRA OF ACETYLENE-HYDROGEN VAN DER WAALS COMPLEX. , 2016, , .		0
21	HIGH-ACCURATE INTERMOLECULAR POTENTIAL ENERGY SURFACE OF HCNâ^'H2 COMPLEX WITH INTRAMOLECULAR VIBRATIONAL MODE OF HCN INCLUDED. , 2016, , .		0
22	FIT POINT-WISE AB INITIO CALCULATION POTENTIAL ENERGIES TO A MULTI-DIMENSION MORSE/LONG-RANGE MODEL. , 2016, , .		0