Jan Kubelka

List of Publications by Year
in descending order

Version: 2024-02-01

78 papers	5,133 citations	126907 33 h-index	85541 71 g-index
80 all docs	80 docs citations	80 times ranked	4374 citing authors

#	Article	IF	Citations
1	Surfactant-induced wettability reversal on oil-wet calcite surfaces: Experimentation and molecular dynamics simulations with scaled-charges. Journal of Colloid and Interface Science, 2022, 609, 890-900.	9.4	16
2	Multi-Probe Equilibrium Analysis of Gradual (Un)Folding Processes. Methods in Molecular Biology, 2022, 2376, 161-171.	0.9	0
3	Liquidâ€“Vapor Interfacial Tension in Alkane Mixtures: Improving Predictive Capabilities of Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2022, 126, 1136-1146.	2.6	3
4	Wettability reversal on oil-wet calcite surfaces: Experimental and computational investigations of the effect of the hydrophobic chain length of cationic surfactants. Journal of Colloid and Interface Science, 2022, 619, 168-178.	9.4	9
5	Wettability Reversal on Dolomite Surfaces by Divalent Ions and Surfactants: An Experimental and Molecular Dynamics Simulation Study. Langmuir, 2021, 37, 6641-6649.	3.5	20
6	Molecular Dynamics Simulations of the Vaporâ€“Liquid Equilibria in CO₂/n-Pentane, Propane/n-Pentane, and Propane/n-Hexane Binary Mixtures. Journal of Physical Chemistry B, 2021, 125, 6658-6669.	2.6	11
7	Wettability alteration by Smart Water multi-ion exchange in carbonates: A molecular dynamics simulation study. Journal of Molecular Liquids, 2021, 332, 115830.	4.9	18
8	Effects of Surfactant Charge and Molecular Structure on Wettability Alteration of Calcite: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 1293-1305.	2.6	21
9	Double Hydrogen Bonding Dimerization Propensity of Aqueous Hydroxy Acids Investigated Using Vibrational Optical Activity. Journal of Physical Chemistry B, 2021, 125, 11350-11363.	2.6	9
10	The effect of molecular isomerism on the induced circular dichroism of cadmium sulfide quantum dots. Journal of Materials Chemistry C, 2021, 9, 17483-17495.	5.5	5
11	Toward the Rational Design of Chemical Formulations for EOR from Carbonates: Molecularâ€“Level Understanding of Carbonate Wettability and its Reversal by Surfactants and Ions. , 2021, , .		0
12	Relationship between molecular charge distribution and wettability reversal efficiency of cationic surfactants on calcite surfaces. Journal of Molecular Liquids, 2020, 318, 114009.	4.9	13
13	Atomistic Molecular Dynamics Simulations of Surfactant-Induced Wettability Alteration in Crevices of Calcite Nanopores. Energy & Fuels, 2020, 34, 3135-3143.	5.1	20
14	Functional Nanoassemblies with Mirror-Image Chiroptical Properties Templated by a Single Homochiral DNA Strand. Chemistry of Materials, 2020, 32, 2272-2281.	6.7	10
15	A positively charged calcite surface model for molecular dynamics studies of wettability alteration. Journal of Colloid and Interface Science, 2020, 569, 128-139.	9.4	33
16	Hydrogen gas formation from the photolysis of rhenium hydrides â€“ mechanistic and computational studies. Dalton Transactions, 2019, 48, 16148-16152.	3.3	1
17	Solid Parahydrogen Infrared Matrix Isolation and Computational Studies of Li_nâ€“(C₂H₄)_m Complexes. Journal of Physical Chemistry A, 2018, 122, 985-991.	2.5	1
18	A new parameterâ€rich structureâ€aware mechanistic model for amino acid substitution during evolution. Proteins: Structure, Function and Bioinformatics, 2018, 86, 218-228.	2.6	8

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19	Effect of Mutations on the Global and Site-Specific Stability and Folding of an Elementary Protein Structural Motif. Journal of Physical Chemistry B, 2018, 122, 11083-11094.	2.6	3
20	Activation Strain Analysis of S_N2 Reactions at C, N, O, and F Centers. Journal of Physical Chemistry A, 2017, 121, 885-891.	2.5	29
21	CdSe Quantum Dots Functionalized with Chiral, Thiol-Free Carboxylic Acids: Unraveling Structural Requirements for Ligand-Induced Chirality. ACS Nano, 2017, 11, 9846-9853.	14.6	55
22	Double Hydrogen Bonding between Side Chain Carboxyl Groups in Aqueous Solutions of Poly (Î²-L-Malic) Tj ETQq0 0 0 rgBT /Overlock 10	2.4	15
23	Chirality Inversion of CdSe and CdS Quantum Dots without Changing the Stereochemistry of the Capping Ligand. ACS Nano, 2016, 10, 3809-3815.	14.6	94
24	Temperature dependence of peptide carboxylic group IR spectra in the amide Iâ€² region at neutral and acidic pH. Vibrational Spectroscopy, 2015, 77, 40-50.	2.2	3
25	Temperature dependence of C-terminal carboxylic group IR absorptions in the amide Iâ€² region. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 134, 473-483.	3.9	4
26	Sequence, structure, and cooperativity in folding of elementary protein structural motifs. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 9890-9895.	7.1	22
27	The N-terminal Domain Allosterically Regulates Cleavage and Activation of the Epithelial Sodium Channel. Journal of Biological Chemistry, 2014, 289, 23029-23042.	3.4	12
28	Temperature dependence of amino acid side chain IR absorptions in the amide I' region. Biopolymers, 2014, 101, 536-548.	2.4	7
29	Site-Specific Thermodynamic Stability and Unfolding of a de Novo Designed Protein Structural Motif Mapped by ¹³C Isotopically Edited IR Spectroscopy. Journal of the American Chemical Society, 2014, 136, 6037-6048.	13.7	25
30	Supramolecular ssDNA Templated Porphyrin and Metalloporphyrin Nanoassemblies with Tunable Helicity. Chemistry - A European Journal, 2014, 20, 1878-1892.	3.3	33
31	Infrared, Vibrational Circular Dichroism, and Raman Spectral Simulations for Î²-Sheet Structures with Various Isotopic Labels, Interstrand, and Stacking Arrangements Using Density Functional Theory. Journal of Physical Chemistry B, 2013, 117, 10343-10358.	2.6	63
32	Structural Analyses of Experimental ¹³C Edited Amide Iâ€² IR and VCD for Peptide Î²-Sheet Aggregates and Fibrils Using DFT-Based Spectral Simulations. Journal of Physical Chemistry B, 2013, 117, 10359-10369.	2.6	33
33	Multivariate Analysis of Spectral Data with Frequency Shifts: Application to Temperature Dependent Infrared Spectra of Peptides and Proteins. Analytical Chemistry, 2013, 85, 9588-9595.	6.5	8
34	Ligand Induced Circular Dichroism and Circularly Polarized Luminescence in CdSe Quantum Dots. ACS Nano, 2013, 7, 11094-11102.	14.6	245
35	Insight into the Packing Pattern of Î²₂ Fibrils: A Model Study of Glutamic Acid Rich Oligomers with ¹³C Isotopic Edited Vibrational Spectroscopy. Biomacromolecules, 2013, 14, 3880-3891.	5.4	34
36	Formation and helicity control of ssDNA templated porphyrin nanoassemblies. Chemical Communications, 2013, 49, 1020-1022.	4.1	36

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37	Effect of Asphaltene Structure on Association and Aggregation Using Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 5765-5776.	2.6	277
38	DFT-Based Simulations of Amide Iâ€² IR Spectra of a Small Protein in Solution Using Empirical Electrostatic Map with a Continuum Solvent Model. Journal of Physical Chemistry B, 2012, 116, 10739-10747.	2.6	7
39	A Phylogenetic Analysis of Normal Modes Evolution in Enzymes and Its Relationship to Enzyme Function. Journal of Molecular Biology, 2012, 422, 442-459.	4.2	22
40	Simulations of the Temperature Dependence of Amide I Vibration. Journal of Physical Chemistry A, 2011, 115, 30-34.	2.5	18
41	Theoretical Modeling of Peptide Î±-Helical Circular Dichroism in Aqueous Solution. Journal of Physical Chemistry A, 2011, 115, 1734-1742.	2.5	31
42	Temperature Effects on the Optical Path Length of Infrared Liquid Transmission Cells. Applied Spectroscopy, 2011, 65, 1307-1313.	2.2	8
43	Fast Side Chain Replacement in Proteins Using a Coarse-Grained Approach for Evaluating the Effects of Mutation During Evolution. Journal of Molecular Evolution, 2011, 73, 23-33.	1.8	5
44	Dynamics of protein folding: Probing the kinetic network of foldingâ€“unfolding transitions with experiment and theory. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1001-1020.	2.3	51
45	DFT-Based Simulations of IR Amide Iâ€² Spectra for a Small Protein in Solution. Comparison of Explicit and Empirical Solvent Models. Journal of Physical Chemistry B, 2010, 114, 13011-13020.	2.6	28
46	Theoretical Study of Vibrationally Averaged Dipole Moments for the Ground and Excited Cî•Ō Stretching States of trans-Formic Acid. Journal of Chemical Theory and Computation, 2010, 6, 817-827.	5.3	8
47	Single-molecule spectroscopy of the temperature-induced collapse of unfolded proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20740-20745.	7.1	211
48	Beyond the nearestâ€neighbor Zimmâ€“Bragg model for helixâ€coil transition in peptides. Biopolymers, 2009, 91, 120-131.	2.4	9
49	On the temperature dependence of amide I intensities of peptides in solution. Vibrational Spectroscopy, 2009, 50, 2-9.	2.2	33
50	Simulation of Vibrational Spectra of Large Molecules by Arbitrary Time Propagation. Journal of Chemical Theory and Computation, 2009, 5, 200-207.	5.3	8
51	Time-resolved methods in biophysics. 9. Laser temperature-jump methods for investigating biomolecular dynamics. Photochemical and Photobiological Sciences, 2009, 8, 499-512.	2.9	62
52	Estimating Free-Energy Barrier Heights for an Ultrafast Folding Protein from Calorimetric and Kinetic Data. Journal of Physical Chemistry B, 2008, 112, 5938-5949.	2.6	78
53	Site-Specific Unfolding Thermodynamics of a Helix-Turn-Helix Protein. Journal of the American Chemical Society, 2008, 130, 8146-8147.	13.7	31
54	Chemical, physical, and theoretical kinetics of an ultrafast folding protein. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 18655-18662.	7.1	141

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55	Cross-Strand Coupling of a Î²-Hairpin Peptide Stabilized with an Aib-Gly Turn Studied Using Isotope-Edited IR Spectroscopy. Journal of the American Chemical Society, 2007, 129, 13592-13603.	13.7	41
56	Infrared and Vibrational CD Spectra of Partially Solvated Î±-Helices:Â DFT-Based Simulations with Explicit Solvent. Journal of Physical Chemistry B, 2007, 111, 1834-1845.	2.6	28
57	On the Temperature Dependence of Amide I Frequencies of Peptides in Solution. Journal of Physical Chemistry B, 2007, 111, 9993-9998.	2.6	44
58	Relaxation Rate for an Ultrafast Folding Protein Is Independent of Chemical Denaturant Concentration. Journal of the American Chemical Society, 2007, 129, 14564-14565.	13.7	41
59	Simulation of Infrared Spectra for Î²-Hairpin Peptides Stabilized by an Aib-Gly Turn Sequence:Â Correlation between Conformational Fluctuation and Vibrational Coupling. Journal of Physical Chemistry B, 2006, 110, 23590-23602.	2.6	29
60	Sub-microsecond Protein Folding. Journal of Molecular Biology, 2006, 359, 546-553.	4.2	232
61	Specificity of the Initial Collapse in the Folding of the Cold Shock Protein. Journal of Molecular Biology, 2006, 360, 1067-1080.	4.2	53
62	Contribution of transition dipole coupling to amide coupling in IR spectra of peptide secondary structures. Vibrational Spectroscopy, 2006, 42, 63-73.	2.2	49
63	IR Study of Cross-Strand Coupling in a Î²-Hairpin Peptide Using Isotopic Labels. Journal of the American Chemical Society, 2005, 127, 4992-4993.	13.7	68
64	Determination of Ultrafast Protein Folding Rates from Loop Formation Dynamics. Journal of Molecular Biology, 2005, 347, 657-664.	4.2	70
65	High-resolution x-ray crystal structures of the villin headpiece subdomain, an ultrafast folding protein. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 7517-7522.	7.1	208
66	Solvent Effects on IR and VCD Spectra of Helical Peptides:Â DFT-Based Static Spectral Simulations with Explicit Water. Journal of Physical Chemistry B, 2005, 109, 8231-8243.	2.6	98
67	The protein folding â€˜speed limitâ€™. Current Opinion in Structural Biology, 2004, 14, 76-88.	5.7	815
68	Nature of Vibrational Coupling in Helical Peptides:Â An Isotopic Labeling Study. Journal of the American Chemical Society, 2004, 126, 2346-2354.	13.7	151
69	Experimental Tests of Villin Subdomain Folding Simulations. Journal of Molecular Biology, 2003, 329, 625-630.	4.2	240
70	Optical Spectroscopic Investigations of Model Î²-Sheet Hairpins in Aqueous Solution. Journal of the American Chemical Society, 2003, 125, 7562-7574.	13.7	104
71	Discrimination between Peptide 310- and Î±-Helices. Theoretical Analysis of the Impact of Î±-Methyl Substitution on Experimental Spectra. Journal of the American Chemical Society, 2002, 124, 5325-5332.	13.7	96
72	Chirality in Peptide Vibrations: Ab Initio Computational Studies of Length, Solvation, Hydrogen Bond, Dipole Coupling, and Isotope Effects on Vibrational CD. ACS Symposium Series, 2002, , 50-64.	0.5	25

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73	Ab Initio Calculation of Amide Carbonyl Stretch Vibrational Frequencies in Solution with Modified Basis Sets. 1. N-Methyl Acetamide. Journal of Physical Chemistry A, 2001, 105, 10922-10928.	2.5	184
74	Differentiation of Î²-Sheet-Forming Structures:Â Ab Initio-Based Simulations of IR Absorption and Vibrational CD for Model Peptide and Protein Î²-Sheets. Journal of the American Chemical Society, 2001, 123, 12048-12058.	13.7	295
75	The Anomalous Infrared Amide I Intensity Distribution in13C Isotopically Labeled Peptide Î²-Sheets Comes from Extended, Multiple-Stranded Structures. An ab Initio Study. Journal of the American Chemical Society, 2001, 123, 6142-6150.	13.7	148
76	Simulations of oligopeptide vibrational CD: Effects of isotopic labeling. Biopolymers, 2000, 53, 380-395.	2.4	73
77	Novel Use of a Static Modification of Two-Dimensional Correlation Analysis. Part I: Comparison of the Secondary Structure Sensitivity of Electronic Circular Dichroism, FT-IR, and Raman Spectra of Proteins. Applied Spectroscopy, 1999, 53, 655-665.	2.2	53
78	Novel Use of a Static Modification of Two-Dimensional Correlation Analysis. Part II: Hetero-Spectral Correlations of Protein Raman, FT-IR, and Circular Dichroism Spectra. Applied Spectroscopy, 1999, 53, 666-671.	2.2	38