Jan Kubelka

List of Publications by Year
in descending order

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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	The protein folding â€˜speed limitâ€™. Current Opinion in Structural Biology, 2004, 14, 76-88.	5.7	815
2	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
3	Effect of Asphaltene Structure on Association and Aggregation Using Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 5765-5776.	2.6	277
4	Ligand Induced Circular Dichroism and Circularly Polarized Luminescence in CdSe Quantum Dots. ACS Nano, 2013, 7, 11094-11102.	14.6	245
5	Experimental Tests of Villin Subdomain Folding Simulations. Journal of Molecular Biology, 2003, 329, 625-630.	4.2	240
6	Sub-microsecond Protein Folding. Journal of Molecular Biology, 2006, 359, 546-553.	4.2	232
7	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
8	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
9	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
10	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
11	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
12	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
13	Optical Spectroscopic Investigations of Model Î²-Sheet Hairpins in Aqueous Solution. Journal of the American Chemical Society, 2003, 125, 7562-7574.	13.7	104
14	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
15	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
16	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
17	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
18	Simulations of oligopeptide vibrational CD: Effects of isotopic labeling. Biopolymers, 2000, 53, 380-395.	2.4	73

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19	Determination of Ultrafast Protein Folding Rates from Loop Formation Dynamics. Journal of Molecular Biology, 2005, 347, 657-664.	4.2	70
20	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
21	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
22	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
23	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
24	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
25	Specificity of the Initial Collapse in the Folding of the Cold Shock Protein. Journal of Molecular Biology, 2006, 360, 1067-1080.	4.2	53
26	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
27	Contribution of transition dipole coupling to amide coupling in IR spectra of peptide secondary structures. Vibrational Spectroscopy, 2006, 42, 63-73.	2.2	49
28	On the Temperature Dependence of Amide I Frequencies of Peptides in Solution. Journal of Physical Chemistry B, 2007, 111, 9993-9998.	2.6	44
29	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
30	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
31	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
32	Formation and helicity control of ssDNA templated porphyrin nanoassemblies. Chemical Communications, 2013, 49, 1020-1022.	4.1	36
33	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
34	On the temperature dependence of amide I intensities of peptides in solution. Vibrational Spectroscopy, 2009, 50, 2-9.	2.2	33
35	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
36	Supramolecular ssDNA Templated Porphyrin and Metalloporphyrin Nanoassemblies with Tunable Helicity. Chemistry - A European Journal, 2014, 20, 1878-1892.	3.3	33

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37	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
38	Site-Specific Unfolding Thermodynamics of a Helix-Turn-Helix Protein. Journal of the American Chemical Society, 2008, 130, 8146-8147.	13.7	31
39	Theoretical Modeling of Peptide Î±-Helical Circular Dichroism in Aqueous Solution. Journal of Physical Chemistry A, 2011, 115, 1734-1742.	2.5	31
40	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
41	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
42	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
43	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
44	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
45	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
46	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
47	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
48	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
49	Atomistic Molecular Dynamics Simulations of Surfactant-Induced Wettability Alteration in Crevices of Calcite Nanopores. Energy & Fuels, 2020, 34, 3135-3143.	5.1	20
50	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
51	Simulations of the Temperature Dependence of Amide I Vibration. Journal of Physical Chemistry A, 2011, 115, 30-34.	2.5	18
52	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
53	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
54	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

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55	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
56	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
57	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
58	Functional Nanoassemblies with Mirror-Image Chiroptical Properties Templated by a Single Homochiral DNA Strand. Chemistry of Materials, 2020, 32, 2272-2281.	6.7	10
59	Beyond the nearestâ€neighbor Zimmâ€“Bragg model for helixâ€coil transition in peptides. Biopolymers, 2009, 91, 120-131.	2.4	9
60	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
61	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
62	Simulation of Vibrational Spectra of Large Molecules by Arbitrary Time Propagation. Journal of Chemical Theory and Computation, 2009, 5, 200-207.	5.3	8
63	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
64	Temperature Effects on the Optical Path Length of Infrared Liquid Transmission Cells. Applied Spectroscopy, 2011, 65, 1307-1313.	2.2	8
65	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
66	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
67	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
68	Temperature dependence of amino acid side chain IR absorptions in the amide I' region. Biopolymers, 2014, 101, 536-548.	2.4	7
69	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
70	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
71	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
72	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

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73	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
74	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
75	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
76	Hydrogen gas formation from the photolysis of rhenium hydrides â€“ mechanistic and computational studies. Dalton Transactions, 2019, 48, 16148-16152.	3.3	1
77	Multi-Probe Equilibrium Analysis of Gradual (Un)Folding Processes. Methods in Molecular Biology, 2022, 2376, 161-171.	0.9	0
78	Toward the Rational Design of Chemical Formulations for EOR from Carbonates: Moleculaâ€“Level Understanding of Carbonate Wettability and its Reversal by Surfactants and Ions. , 2021, , .		0