Chiara Castiglioni

List of Publications by Year
in descending order

214 papers	6,709 citations	61984 43 h-index	88630 70 g-index
219 all docs	219 docs citations	219 times ranked	6043 citing authors

#	Article	IF	Citations
1	Raman spectroscopy of polyconjugated molecules and materials: confinement effect in one and two dimensions. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2004, 362, 2425-2459.	3.4	248
2	A simple interpretation of the vibrational spectra of undoped, doped and photoexcited polyacetylene: Amplitude mode theory in the GF formalism. Solid State Communications, 1988, 65, 625-630.	1.9	221
3	Common force field for graphite and polycyclic aromatic hydrocarbons. Physical Review B, 1999, 60, 12710-12725.	3.2	201
4	Confinement potential and Ï€-electron delocalization in polyconjugated organic materials. Physical Review B, 1994, 50, 9815-9823.	3.2	184
5	Biradicaloid and Polyenic Character of Quinoidal Oligothiophenes Revealed by the Presence of a Low-Lying Double-Exciton State. Journal of Physical Chemistry Letters, 2010, 1, 3334-3339.	4.6	150
6	Vibrational Raman spectroscopy of polyconjugated organic oligomers and polymers. Journal of Raman Spectroscopy, 1993, 24, 485-494.	2.5	143
7	Origin of the D line in the Raman spectrum of graphite: A study based on Raman frequencies and intensities of polycyclic aromatic hydrocarbon molecules. Journal of Chemical Physics, 2001, 114, 963.	3.0	140
8	Raman activation in disordered graphites of the A1â€² symmetry forbidden kâ‰0 phonon: The origin of the D line. Journal of Chemical Physics, 2001, 115, 3769-3778.	3.0	133
9	A Computational Study of the Raman Spectra of Large Polycyclic Aromatic Hydrocarbons:â€‰ Toward Molecularly Defined Subunits of Graphite. Journal of Physical Chemistry A, 2002, 106, 3306-3317.	2.5	131
10	Molecular first hyperpolarizability of push-pull polyenes: Relationship between electronic and vibrational contribution by a two-state model. Physical Review B, 1996, 53, 13319-13325.	3.2	128
11	Infrared intensities: from intensity parameters to an overall understanding of the spectrum. Journal of Molecular Structure, 1990, 224, 445-470.	3.6	122
12	Infrared intensities. Use of the CH-stretching band intensity as a tool for evaluating the acidity of hydrogen atoms in hydrocarbons. Journal of Molecular Structure, 2000, 521, 1-18.	3.6	121
13	Physical meaning of electrooptical parameters derived from infrared intensities. The Journal of Physical Chemistry, 1984, 88, 600-604.	2.9	114
14	Probing the structure of polymer blends by vibrational spectroscopy: the case of poly(ethylene oxide) and poly(methyl methacrylate) blends. Polymer, 1985, 26, 811-820.	3.8	111
15	Raman and SERS investigation of isolated sp carbon chains. Chemical Physics Letters, 2006, 417, 78-82.	2.6	102
16	Quantum-Chemical Insights into the Prediction of Charge Transport Parameters for a Naphthalenetetracarboxydiimide-Based Copolymer with Enhanced Electron Mobility. Journal of the American Chemical Society, 2011, 133, 19056-19059.	13.7	95
17	A C216-Nanographene Molecule with Defined Cavity as Extended Coronoid. Journal of the American Chemical Society, 2016, 138, 4322-4325.	13.7	90
18	Resonance Raman contribution to the D band of carbon materials: Modeling defects with quantum chemistry. Journal of Chemical Physics, 2004, 120, 11889-11900.	3.0	87

#	Article	IF	Citations
19	Resistive Molecular Memories: Influence of Molecular Parameters on the Electrical Bistability. Journal of the American Chemical Society, 2009, 131, 6591-6598.	13.7	86
20	Relaxation contribution to hyperpolarizability. A semiclassical model. Solid State Communications, 1992, 82, 13-17.	1.9	83
21	Ab initio counterpart of infrared atomic charges. Chemical Physics Letters, 1987, 142, 515-518.	2.6	69
22	A molecular viewpoint of lattice dynamics and spectra of conducting polymers. Synthetic Metals, 1989, 28, D359-D368.	3.9	69
23	Solvent effects on firstâ€order molecular hyperpolarizability: A study based on vibrational observables. Journal of Chemical Physics, 1995, 103, 9935-9940.	3.0	66
24	P(VDF-TrFE) nanofibers: structure of the ferroelectric and paraelectric phases through IR and Raman spectroscopies. RSC Advances, 2020, 10, 37779-37796.	3.6	65
25	Vibrational Spectroscopy of Polyconjugated Aromatic Materials with Electrical and Non Linear Optical Properties. , 1991, , 435-507.		64
26	Molecular Level Investigation of the Film Structure of a High Electron Mobility Copolymer via Vibrational Spectroscopy. Macromolecules, 2013, 46, 2658-2670.	4.8	63
27	Graphite and graphitic compounds: vibrational spectra from oligomers to real materials. Journal of Molecular Structure, 1999, 480-481, 615-620.	3.6	62
28	Ab Initio Calculation of the IR Spectrum of PTFE: Helical Symmetry and Defects. Journal of Physical Chemistry B, 2013, 117, 706-718.	2.6	60
29	Color polymorphism in organic crystals. Communications Chemistry, 2020, 3, .	4.5	60
30	Carbon nanowires: Phonon andÏ€-electron confinement. Physical Review B, 2006, 74, .	3.2	59
31	Tuning the Quinoid versus Biradicaloid Character of Thiophene-Based Heteroquaterphenoquinones by Means of Functional Groups. Journal of the American Chemical Society, 2012, 134, 19070-19083.	13.7	59
32	Relationship between infrared and Raman intensities in molecules with polarized Ï€ electrons. Journal of Molecular Structure, 1999, 480-481, 179-188.	3.6	57
33	Experimental molecular hyperpolarizabilities from vibrational spectra in systems with large electron-phonon coupling. Synthetic Metals, 1995, 74, 171-177.	3.9	56
34	Ab Initio Calculation of the Crystalline Structure and IR Spectrum of Polymers: Nylon 6 Polymorphs. Journal of Physical Chemistry B, 2012, 116, 8299-8311.	2.6	56
35	Intramolecular electrical and dynamical interactions in formaldehyde: A discussion based on infrared intensity data. Journal of Chemical Physics, 1985, 82, 3534-3541.	3.0	54
36	Adding Four Extra K-Regions to Hexa-peri-hexabenzocoronene. Journal of the American Chemical Society, 2016, 138, 4726-4729.	13.7	52

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37	Stabilization of linear carbon structures in a solid Ag nanoparticle assembly. Applied Physics Letters, 2007, 90, 013111.	3.3	50
38	Structure and chain polarization of long polyynes investigated with infrared and Raman spectroscopy. Journal of Raman Spectroscopy, 2013, 44, 1398-1410.	2.5	50
39	A relationship between Raman and infrared spectra: the case of pushâ€“pull molecules. Chemical Physics Letters, 1998, 287, 100-108.	2.6	48
40	Charge distribution from infrared intensities: Charges on hydrogen atoms and hydrogen bond. Journal of Chemical Physics, 1984, 80, 1377-1381.	3.0	46
41	Ï€-Conjugation and End Group Effects in Long Cumulenes: Raman Spectroscopy and DFT Calculations. Journal of Physical Chemistry C, 2014, 118, 26415-26425.	3.1	46
42	Intramolecular Vibrational Force Fields for Linear Carbon Chains through an Adaptative Linear Scaling Scheme. Journal of Physical Chemistry A, 2007, 111, 11645-11651.	2.5	45
43	Wavelength-dependent Raman activity of D2h symmetry polycyclic aromatic hydrocarbons in the D-band and acoustic phonon regions. Chemical Physics, 2004, 301, 81-93.	1.9	43
44	Firstâ€principles calculation of the Peierls distortion in an infinite linear carbon chain: the contribution of Raman spectroscopy. Journal of Raman Spectroscopy, 2008, 39, 164-168.	2.5	43
45	Biradicaloid Character of Thiopheneâ€Based Heterophenoquinones: The Role of Electronâ€“Phonon Coupling. ChemPhysChem, 2010, 11, 3685-3695.	2.1	43
46	Bottomâ€Up Synthesis of Necklaceâ€Like Graphene Nanoribbons. Chemistry - an Asian Journal, 2015, 10, 2134-2138.	3.3	43
47	Disclosing the Early Stages of Electrochemical Anion Intercalation in Graphite by a Combined Atomic Force Microscopy/Scanning Tunneling Microscopy Approach. Journal of Physical Chemistry C, 2016, 120, 6088-6093.	3.1	43
48	Characteristic infrared intensities of CH bonds. Journal of Molecular Structure, 1986, 141, 341-346.	3.6	41
49	A joint Raman and EPR spectroscopic study on ball-milled nanographites. Chemical Physics Letters, 2011, 516, 220-224.	2.6	41
50	Overtone and combination features of G and D peaks in resonance Raman spectroscopy of the C₇₈H₂₆ polycyclic aromatic hydrocarbon. Journal of Raman Spectroscopy, 2015, 46, 757-764.	2.5	41
51	sp Carbon chain interaction with silver nanoparticles probed by Surface Enhanced Raman Scattering. Chemical Physics Letters, 2009, 478, 45-50.	2.6	40
52	Modeling of Molecular Charge Distribution on the Basis of Experimental Infrared Intensities and First-Principles Calculations: The Case of CH Bonds. Journal of Physical Chemistry A, 2010, 114, 624-632.	2.5	40
53	Raman scattering of molecular graphenes. Physical Chemistry Chemical Physics, 2009, 11, 10185.	2.8	39
54	Molecular Hyperpolarizabilities from Vibrational Spectroscopy: Polyenovanillins. The Journal of Physical Chemistry, 1995, 99, 16242-16247.	2.9	38

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55	Solid-state synthesis of mixed trihalides via reversible absorption of dihalogens by non porous onium salts. CrystEngComm, 2011, 13, 4427.	2.6	38
56	Derivation of charge distribution from infrared intensities: The case of polyacetylene. Spectrochimica Acta Part A: Molecular Spectroscopy, 1985, 41, 371-380.	0.1	37
57	Ab initio counterpart of infrared atomic charges. Comparison with charges obtained from electrostatic potentials. Chemical Physics Letters, 1988, 151, 397-402.	2.6	37
58	Ab initio counterpart of infrared atomic charges: Charge fluxes. Chemical Physics Letters, 1989, 160, 200-205.	2.6	36
59	Anthracene/tetracene cocrystals as novel fluorophores in thin-film luminescent solar concentrators. RSC Advances, 2014, 4, 9893.	3.6	35
60	Formation of weak hydrogen-bonded complexes as predicted by experimental atomic charges. Chemical Physics Letters, 1983, 99, 101-106.	2.6	34
61	Non-linear optical response to strong applied electromagnetic fields in polyconjugated materials. Synthetic Metals, 1992, 51, 135-146.	3.9	34
62	Experimental vibrational contributions to molecular hyperpolarisabilities: methods and measurements. Journal of Molecular Structure, 2000, 521, 137-155.	3.6	34
63	Spectroscopic studies and first-principles modelling of 2,2,4-trifluoro-5-trifluoromethoxy-1,3-dioxole (TTD) and TTDâ€“TFE copolymers (HyflonÂ® AD). Polymer, 2008, 49, 1812-1822.	3.8	34
64	Density functional theory prediction of the vibrational spectra of polycyclic aromatic hydrocarbons: effect of molecular symmetry and size on Raman intensities. Journal of Molecular Structure, 2001, 563-564, 79-87.	3.6	33
65	A simple way to obtain information on charge distribution in molecules directly from infrared spectra: the case of Cî—¸H bonds. Journal of Molecular Structure, 1989, 198, 475-488.	3.6	32
66	Multi-wavelength Raman response of disordered graphitic materials: models and simulations. Synthetic Metals, 2003, 139, 885-888.	3.9	32
67	IR spectroscopy of crystalline polymers from ab initio calculations: Nylon 6,6. Vibrational Spectroscopy, 2013, 66, 83-92.	2.2	32
68	Effect of bond length alternation and of bond length alternation oscillations on the molecular nonlinear optical response of push pull polyenes. Journal of the Optical Society of America B: Optical Physics, 1998, 15, 308.	2.1	31
69	Ag and Au nanoparticles for SERS substrates produced by pulsed laser ablation. Crystal Research and Technology, 2011, 46, 836-840.	1.3	31
70	Joint Experimental and Computational Investigation of the Structural and Spectroscopic Properties of Poly(vinylidene fluoride) Polymorphs. Journal of Physical Chemistry B, 2015, 119, 4888-4897.	2.6	31
71	Use of vibrational spectra for the determination of first-order molecular hyperpolarizabilities of push-pull polyenes as function of structural parameters. Journal of Applied Polymer Science, 1998, 70, 1311-1320.	2.6	30
72	Hyperconjugation from infrared intensities: the case of methyl acetate and of its selectively deuterated derivatives. Journal of Molecular Structure, 1994, 324, 189-198.	3.6	29

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73	Î¼â€Raman mapping to study calcium oxalate historical films. Journal of Raman Spectroscopy, 2012, 43, 1604-1611.	2.5	29
74	Experimental atomic charges from infrared intensities. Comparison with â€œab initioâ€•values. Chemical Physics Letters, 1983, 95, 483-485.	2.6	28
75	Charge mobility in Ïƒâ€bonded molecules: The infrared spectrum of polymethylene chains in the solid and liquid phases. Journal of Chemical Physics, 1991, 95, 7144-7149.	3.0	28
76	Nuclear contribution to hyperpolarizability of polyconjugated compounds: role of vibrational intensities. Synthetic Metals, 1993, 57, 3919-3926.	3.9	28
77	Stabilization energies of weak hydrogen bonded molecular complexes. Comparison of simple models. Journal of Chemical Physics, 1984, 80, 3916-3918.	3.0	27
78	Atomic charges from atomic polar tensors: A comparison of methods. Computational and Theoretical Chemistry, 2010, 955, 158-164.	1.5	27
79	Biobased Janus molecule for the facile preparation of water solutions of few layer graphene sheets. RSC Advances, 2015, 5, 81142-81152.	3.6	27
80	Can Raman spectroscopy detect cumulenic structures of linear carbon chains?. Journal of Raman Spectroscopy, 2010, 41, 226-236.	2.5	26
81	Vibrational overtones quenching of near infrared emission in Er3+ complexes. New Journal of Chemistry, 2009, 33, 1542.	2.8	26
82	Coarseâ€Grained Simulations of Model Polymer Nanofibres. Macromolecular Theory and Simulations, 2011, 20, 305-319.	1.4	26
83	Diamond graphitization by laser-writing for all-carbon detector applications. Diamond and Related Materials, 2017, 75, 25-33.	3.9	26
84	Peierls distortion in trans polyacetylene: Evidence from infrared intensities. Solid State Communications, 1985, 56, 863-866.	1.9	25
85	Infrared intensities and charge mobility in hydrogen bonded complexes. Journal of Chemical Physics, 2013, 139, 074304.	3.0	25
86	Polaron Confinement in n-Doped P(NDI2OD-T2) Unveiled by Vibrational Spectroscopy. Chemistry of Materials, 2019, 31, 6726-6739.	6.7	25
87	Charge fluxes and electron delocalization in conducting polymers from infrared intensities. Synthetic Metals, 1987, 17, 293-300.	3.9	24
88	High purity multiwalled carbon nanotubes under high pressure and high temperature. Carbon, 2003, 41, 2361-2367.	10.3	24
89	Atomic charges from IR intensity parameters: theory, implementation and application. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	24
90	Microscopic Analysis of the Different Perchlorate Anions Intercalation Stages of Graphite. Journal of Physical Chemistry C, 2017, 121, 14246-14253.	3.1	23

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91	Vibrational Analysis as a Tool for Detecting Electronic Mobility. The Case of the Alternating Ethylene-Tetrafluoroethylene Copolymers. Macromolecules, 1994, 27, 2194-2199.	4.8	22
92	Environmental degradation of a novel ethyleneâ€“propylene copolymer in thick sheets. European Polymer Journal, 2005, 41, 359-366.	5.4	22
93	Assignment of theG+andGâ^'Raman bands of metallic and semiconducting carbon nanotubes based on a common valence force field. Physical Review B, 2006, 74, .	3.2	22
94	Modulation of the Refractive Index by Photoisomerization of Diarylethenes: Theoretical Modeling. Journal of Physical Chemistry A, 2008, 112, 7473-7480.	2.5	22
95	Evolution of the graphite surface in phosphoric acid: an AFM and Raman study. Beilstein Journal of Nanotechnology, 2016, 7, 1878-1884.	2.8	22
96	Combining Static and Dynamical Approaches for Infrared Spectra Calculations of Gas Phase Molecules and Clusters. Journal of Chemical Theory and Computation, 2017, 13, 3802-3813.	5.3	22
97	Domino Reaction for the Sustainable Functionalization of Few-Layer Graphene. Nanomaterials, 2019, 9, 44.	4.1	22
98	Understanding of vibrational spectra of polyconjugated molecules by means of the â€œeffective conjugation coordinateâ€• Synthetic Metals, 1991, 43, 3407-3412.	3.9	21
99	Molecular charge distribution and charge fluxes from Atomic Polar Tensors: The case of OH bonds. Journal of Molecular Structure, 2010, 976, 342-349.	3.6	21
100	Hydrogen bonding effects in perfluorinated polyamides: An investigation based on infrared spectroscopy and density functional theory calculations. Polymer, 2010, 51, 2597-2610.	3.8	20
101	Predictive modeling of the vibrational quenching in emitting lanthanides complexes. Synthetic Metals, 2012, 161, 2693-2699.	3.9	20
102	A Novel Classification Method for Multispectral Imaging Combined with Portable Raman Spectroscopy for the Analysis of a Painting by Vincent Van Gogh. Applied Spectroscopy, 2013, 67, 1234-1241.	2.2	20
103	Modeling phonons of carbon nanowires. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 2570-2576.	2.7	19
104	Charge mobility in molecules: Charge fluxes from second derivatives of the molecular dipole. Journal of Chemical Physics, 2013, 138, 164115.	3.0	19
105	Structural Characterization of Highly Oriented Naphthalene-Diimide-Bithiophene Copolymer Films via Vibrational Spectroscopy. Journal of Physical Chemistry B, 2015, 119, 2062-2073.	2.6	19
106	Molecular point charges as derived from infrared intensities and from ab initio calculations. Computational and Theoretical Chemistry, 1986, 138, 203-212.	1.5	18
107	Amplitude mode theory and classical molecular dynamics: The interpretation of the vibrational infrared and Raman spectra of polyparaphenylene. Synthetic Metals, 1989, 29, 1-6.	3.9	18
108	The trans effect of lone pairs on individual X-H bonds (X = C or N). An ab initio study. Computational and Theoretical Chemistry, 1994, 305, 19-25.	1.5	18

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109	Characterization of Naturally Weathered Polypropylene Plates. Journal of Macromolecular Science - Pure and Applied Chemistry, 2006, 43, 535-554.	2.2	18
110	Incipient Anion Intercalation of Highly Oriented Pyrolytic Graphite Close to the Oxygen Evolution Potential: A Combined X-ray Photoemission and Raman Spectroscopy Study. Journal of Physical Chemistry C, 2019, 123, 1790-1797.	3.1	18
111	Experimental and theoretical molecular force fields of polyenes in the light of the amplitude mode theory. Synthetic Metals, 1989, 28, D375-D380.	3.9	17
112	Edge chlorination of hexa-peri-hexabenzocoronene investigated by density functional theory and vibrational spectroscopy. Physical Chemistry Chemical Physics, 2016, 18, 11869-11878.	2.8	17
113	Chemical pathways in the partial oxidation and steam reforming of acetic acid over a Rh-Al 2 O 3 catalyst. Catalysis Today, 2017, 289, 162-172.	4.4	17
114	Resistive memories based on Rose Bengal and related xanthene derivatives: insights from modeling charge transport properties. Physical Chemistry Chemical Physics, 2010, 12, 1600.	2.8	16
115	Phonon, Ï€ electron localization and size of the charge carrier in paraâ€phenylenevinylene oligomers and polymer: A spectroscopic study. Journal of Chemical Physics, 1996, 105, 2509-2516.	3.0	15
116	Reply to â€œComment on â€˜Molecular first hyperpolarizability of push-pull polyenes: Relationship between electronic and vibrational contribution by a two-state modelâ€™ â€. Physical Review B, 1997, 56, 2275-2276.	3.2	15
117	Tuning the Solubility Parameters of Carbon Nanotubes by Means of Their Adducts with Janus Pyrrole Compounds. Nanomaterials, 2020, 10, 1176.	4.1	15
118	Through bond and through space interactions in oligoâ€“alkoxythiophenes: A spectroscopic study. Journal of Chemical Physics, 1996, 105, 9461-9469.	3.0	14
119	The vibrational approach to determine molecular nonlinearities: What do we learn from the method and the data?. Synthetic Metals, 1997, 85, 1043-1046.	3.9	14
120	Spectroscopic behaviour, bond properties and charge distribution in methoxy groups in hydrofluoroethers: the effect of neighbouring CF2 group. Computational and Theoretical Chemistry, 2004, 710, 151-162.	1.5	14
121	Molecular conformations of a partially halogenated ether: A study based on infrared spectroscopy and density functional theory calculations. Journal of Fluorine Chemistry, 2006, 127, 320-329.	1.7	14
122	Intramolecular and intermolecular OHâ€¦O and OHâ€¦F interactions in perfluoropolyethers with polar end groups: IR spectroscopy and first-principles calculations. European Polymer Journal, 2012, 48, 391-403.	5.4	14
123	Intermolecular modulation of IR intensities in the solid state. The role of weak interactions in polyethylene crystal: A computational DFT study. Journal of Chemical Physics, 2016, 145, 144901.	3.0	14
124	Atomic charges and charge fluxes in cis and trans-C2H2X2 (X=F, Cl): an ab initio study. Journal of Molecular Structure, 1991, 248, 281-288.	3.6	13
125	Relaxing the graphite lattice along critical directions: The effect of the electronâ€“phonon coupling on the Ï€ electron band structure. Chemical Physics Letters, 2005, 414, 166-173.	2.6	13
126	Hydrogen bonding in amylose/DMSO complexes studied by vibrational spectroscopy and density functional theory calculations. Journal of Raman Spectroscopy, 2009, 40, 1110-1116.	2.5	13

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127	Size-selected polyynes synthesised by submerged arc discharge in water. Chemical Physics Letters, 2020, 740, 137054.	2.6	13
128	Exploiting Direct Current Plasma Electrolytic Oxidation to Boost Photoelectrocatalysis. Catalysts, 2020, 10, 325.	3.5	13
129	Raman and IR spectra of graphdiyne nanoribbons. Physical Review Materials, 2020, 4, .	2.4	13
130	On the enhancement of the electric dipole moment in molecular complexes. Journal of Molecular Structure, 1984, 115, 319-322.	3.6	12
131	Characterisation of an inclusion complex between cladribine and 2-hydroxypropyl-β-cyclodextrin**The work described in this article was carried out at Merck Serono SpA, Tiburtina Site, via L. Einaudi 11, 00012 Guidonia Montecelio, Roma, Italy. Some additional measurements were carried out at Dipartimento di Chimica, Materiali e Ingegneria Chimica â€œG. Nattaâ€, Politecnico di Milano, P. za Leonardo da Vinci 32, 20133 Milano, Italy.. Journal of Pharmaceutical Sciences, 2008, 97, 3897-3906.	3.3	12
132	Annular reactor testing and Raman surface characterization in the CPO of methane and propylene. Applied Catalysis A: General, 2014, 474, 149-158.	4.3	12
133	Outside rules inside: the role of electron-active substituents in thiophene-based heterophenoquinones. Physical Chemistry Chemical Physics, 2015, 17, 10426-10437.	2.8	12
134	Annular reactor testing and Raman surface characterization of the CPO of i-octane and n-octane on Rh based catalyst. Chemical Engineering Journal, 2016, 294, 9-21.	12.7	12
135	Experimental Charge Distribution in Polyacetylene. Molecular Crystals and Liquid Crystals, 1985, 117, 295-298.	0.8	11
136	Atomic charges in fluoroethylenes from molecular-orbital calculations and from infrared intensities. Chemical Physics Letters, 1990, 170, 335-344.	2.6	11
137	Stone/Coating Interaction and Durability of Si-Based Photocatalytic Nanocomposites Applied to Porous Lithotypes. Materials, 2018, 11, 2289.	2.9	11
138	Evidence of graphite blister evolution during the anion de-intercalation process in the cathodic regime. Applied Surface Science, 2020, 504, 144440.	6.1	11
139	Vibrational and nonlinear optical properties of amine-capped push-pull polyynes by infrared and Raman spectroscopy. Carbon Trends, 2021, 5, 100115.	3.0	11
140	Stereoelectronic Effects in Polythiophenes. Molecular Crystals and Liquid Crystals, 1993, 236, 181-188.	0.3	10
141	NLO responses of organic materials: The vibrational approach. Advanced Materials, 1996, 8, 345-347.	21.0	10
142	Effective hamiltonian for Ï€ electrons in linear carbon chains. Chemical Physics Letters, 2007, 450, 86-90.	2.6	10
143	Two dimensional correlation Raman spectroscopy of perfluoropolyethers: Effect of peroxide groups. Journal of Molecular Structure, 2010, 974, 73-79.	3.6	10
144	Enhancing the light driven modulation of the refractive index in organic photochromic materials: A quantum chemical strategy. Journal of Photochemistry and Photobiology A: Chemistry, 2010, 214, 61-68.	3.9	10

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145	FT-IR Spectroscopy and DFT Calculations on Fluorinated Macromer Diols: IR Intensity and Association Properties. Journal of Physical Chemistry B, 2010, 114, 6332-6336.	2.6	10
146	Radiolytic degradation of hydrophilic PyTri ligands for minor actinide recycling. Journal of Radioanalytical and Nuclear Chemistry, 2019, 322, 1663-1673.	1.5	10
147	Nonâ€invasive and in situ investigation of layers sequence in panel paintings by portable microâ€spatially offset Raman spectroscopy. Journal of Raman Spectroscopy, 2020, 51, 2016-2021.	2.5	10
148	Raman Fingerprints of Ï€-Electron Delocalization in Polythiophene-Based Insulated Molecular Wires. Macromolecules, 2022, 55, 3458-3468.	4.8	10
149	Charge distribution from infrared intensities: Which CH bonds form hydrogen bonds?. Chemical Physics Letters, 1985, 117, 263-265.	2.6	9
150	New strategies for new organic molecules with large second order hyperpolarizabilities. Journal of the Chemical Society Perkin Transactions II, 1999, , 1765-1770.	0.9	9
151	Infrared Intensity Studies in Fluorinated Macromolecules. Macromolecular Symposia, 2008, 265, 218-224.	0.7	9
152	Radiation-induced modifications on physico chemical properties of diluted nitric acid solutions within advanced spent nuclear fuel reprocessing. Journal of Radioanalytical and Nuclear Chemistry, 2015, 304, 395-400.	1.5	9
153	Non-invasive characterisation of molecular diffusion of agent into turbid matrix using micro-SORS. Talanta, 2020, 218, 121078.	5.5	9
154	The correlation between experimental polarized Raman spectra and their density functional theory prediction in the LCAO framework: The R3c LiNbO₃ crystal as a test case. Journal of Raman Spectroscopy, 2021, 52, 995-1010.	2.5	9
155	Vibrational intensities in molecules with strained bonds: cyclopropane. Canadian Journal of Chemistry, 1985, 63, 2059-2064.	1.1	8
156	FTIR spectra (frequency and intensity) of poly-(para-phenylenes). Mikrochimica Acta, 1988, 94, 247-249.	5.0	8
157	Quantum mechanical calculations and spectroscopic analysis of fluorinated vinyl ether molecules. Journal of Fluorine Chemistry, 1999, 95, 105-116.	1.7	8
158	Resonant Raman spectroscopy of nanostructured carbon-based materials: the molecular approach. AIP Conference Proceedings, 2004, , .	0.4	8
159	Perfluoropoly-ether/peroxide compounds: spectroscopic studies and quantum chemical calculations. Journal of Fluorine Chemistry, 2004, 125, 151-164.	1.7	8
160	Anharmonic overtones quenching in Er3+ complexes. Synthetic Metals, 2009, 159, 2410-2412.	3.9	8
161	Mechanochromic Luminescent Tetrathiazolylthiophenes: Evaluating the Role of Intermolecular Interactions through Pressure and Temperature-Dependent Raman Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 17537-17543.	3.1	8
162	Immobilized Nano-TiO2 Photocatalysts for the Degradation of Three Organic Dyes in Single and Multi-Dye Solutions. Coatings, 2020, 10, 919.	2.6	8

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163	In situ synthesis of polyynes in a polymer matrix via pulsed laser ablation in a liquid. Materials Advances, 2020, 1, 2729-2736.	5.4	8
164	Raman spectroscopy of holey nanographene C216. Journal of Raman Spectroscopy, 2021, 52, 2301-2316.	2.5	8
165	Molecular Aspects, Vibrational Spectroscopy and Dynamics of Polyacetylene. Molecular Crystals and Liquid Crystals, 1985, 117, 287-294.	0.8	7
166	Low-frequency vibrational modes and static vibrational hyperolarizabilities of long-chain molecules: polyenes and polyacetylene. Computational and Theoretical Chemistry, 2000, 500, 323-338.	1.5	7
167	Structure and Electrical Bistability of a New Class of Diphenyl-bithiophenes: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry C, 2008, 112, 18628-18637.	3.1	7
168	Comparison of experimental and â€œab initioâ€•intensity parameters. Journal of Molecular Structure, 1988, 174, 47-52.	3.6	6
169	Intramolecular charge delocalization and nonlinear optical properties from vibrational spectra. Synthetic Metals, 1999, 102, 1582-1583.	3.9	6
170	Outdoor ageing of ethyleneâ€“carbon monoxide alternating copolymer. Polymer Degradation and Stability, 2000, 69, 133-142.	5.8	6
171	A Spectroscopic Approach to Carbon Materials for Energy Storage. , 0, , 23-53.		6
172	Beyond the Continuum Approach. , 0, , 499-605.		6
173	Raman spectroscopic characterization of a thiopheneâ€based active material for resistive organic nonvolatile memories. Journal of Raman Spectroscopy, 2010, 41, 406-413.	2.5	6
174	Physico chemical properties of irradiated i-SANEX diluents. Nukleonika, 2015, 60, 893-898.	0.8	6
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