

# Elisabetta Venuti

## List of Publications by Year in descending order

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114  
papers

3,894  
citations

136950

32  
h-index

133252

59  
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116  
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116  
docs citations

116  
times ranked

3617  
citing authors

#	ARTICLE	IF	CITATIONS
1	A third blind test of crystal structure prediction. <i>Acta Crystallographica Section B: Structural Science</i> , 2005, 61, 511-527.	1.8	373
2	Significant progress in predicting the crystal structures of small organic molecules – a report on the fourth blind test. <i>Acta Crystallographica Section B: Structural Science</i> , 2009, 65, 107-125.	1.8	371
3	Towards crystal structure prediction of complex organic compounds – a report on the fifth blind test. <i>Acta Crystallographica Section B: Structural Science</i> , 2011, 67, 535-551.	1.8	358
4	Peierls and Holstein carrier-phonon coupling in crystalline rubrene. <i>Physical Review B</i> , 2010, 82, .	3.2	113
5	Epitaxial Growth of $\pi$ -Stacked Perfluoropentacene on Graphene-Coated Quartz. <i>ACS Nano</i> , 2012, 6, 10874-10883.	14.6	108
6	Probing polymorphs of organic semiconductors by lattice phonon Raman microscopy. <i>CrystEngComm</i> , 2008, 10, 937.	2.6	103
7	Structure, Stoichiometry, and Charge Transfer in Cocrystals of Perylene with TCNQ-F <sub>x</sub> . <i>Crystal Growth and Design</i> , 2016, 16, 3028-3036.	3.0	99
8	High-pressure densification of silica glass: A molecular-dynamics simulation. <i>Physical Review B</i> , 1996, 54, 3809-3816.	3.2	78
9	Raman phonon spectra of pentacene polymorphs. <i>Chemical Physics Letters</i> , 2002, 357, 32-36.	2.6	77
10	Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene. <i>ChemPhysChem</i> , 2009, 10, 2265-2273.	2.1	77
11	Phonons and structures of tetracene polymorphs at low temperature and high pressure. <i>Physical Review B</i> , 2004, 70, .	3.2	75
12	Characterization of Phase Purity in Organic Semiconductors by Lattice-Phonon Confocal Raman Mapping: Application to Pentacene. <i>Advanced Materials</i> , 2005, 17, 2549-2553.	21.0	67
13	Inherent structures of crystalline pentacene. <i>Journal of Chemical Physics</i> , 2003, 118, 807-815.	3.0	62
14	The four polymorphic modifications of the semiconductor dibenzo-tetrathiafulvalene. <i>CrystEngComm</i> , 2008, 10, 1899.	2.6	62
15	High dimensional anharmonic potential energy surfaces: The case of methane. <i>Journal of Chemical Physics</i> , 1999, 110, 7339-7347.	3.0	58
16	Probing Pentacene Polymorphs by Lattice Dynamics Calculations. <i>Journal of the American Chemical Society</i> , 2002, 124, 2128-2129.	18.7	57
17	Crystal structure of oligoacenes under high pressure. <i>Physical Review B</i> , 2006, 74, .	3.2	56
18	Pressure-induced phase transition in pentacene. <i>Chemical Physics Letters</i> , 2003, 375, 490-494.	2.6	55

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19	Intramolecular and Low-Frequency Intermolecular Vibrations of Pentacene Polymorphs as a Function of Temperature. <i>Journal of Physical Chemistry B</i> , 2004, 108, 1822-1826.	2.6	53
20	Photophysical properties of methylated phenols in nonpolar solvents. <i>The Journal of Physical Chemistry</i> , 1990, 94, 3609-3613.	2.9	50
21	The phototransformation process in phytochrome. I. Ultrafast fluorescence component and kinetic models for the initial Pr <sup>+</sup> Pfr transformation steps in native phytochrome. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 1992, 1140, 59-68.	1.0	50
22	Structure and Morphology of PDI8aCN2 for n-type Thin-Film Transistors. <i>Advanced Functional Materials</i> , 2012, 22, 943-953.	14.9	50
23	Polarized Raman Spectra of a Rubrene Single Crystal. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17416-17422.	3.1	45
24	Interaction of charge carriers with lattice and molecular phonons in crystalline pentacene. <i>Journal of Chemical Physics</i> , 2011, 135, 084701.	3.0	44
25	Vibration-Rotation Spectra of <sup>13</sup> C Containing Acetylene. <i>Journal of Molecular Spectroscopy</i> , 1993, 161, 466-486.	1.2	42
26	DFT-Assisted Polymorph Identification from Lattice Raman Fingerprinting. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3690-3695.	4.6	42
27	A molecular dynamics study of the vibrational properties of silica glass. <i>Chemical Physics</i> , 1994, 179, 411-419.	1.9	40
28	Structure and dynamics of pentacene on SiO <sub>2</sub> : From monolayer to bulk structure. <i>Physical Review B</i> , 2012, 85, ..	3.2	40
29	The vibrational energy pattern in acetylene. V. <sup>13</sup> C <sub>2</sub> H <sub>2</sub> . <i>Journal of Chemical Physics</i> , 1999, 111, 1008-1016.	3.0	37
30	Mechanisms of deactivation of the low-lying electronic states of 2,2'-bipyridine. <i>The Journal of Physical Chemistry</i> , 1990, 94, 1740-1745.	2.9	35
31	Newly developed electrochemical synthesis of Co-based layered double hydroxides: toward noble metal-free electro-catalysis. <i>Journal of Materials Chemistry A</i> , 2019, 7, 11241-11249.	10.3	34
32	Quasi harmonic lattice dynamics: the phase diagram of benzene. <i>Chemical Physics</i> , 1996, 202, 231-241.	1.9	33
33	Quasiharmonic lattice-dynamics and molecular-dynamics calculations for the Lennard-Jones solids. <i>Physical Review B</i> , 1998, 58, 206-212.	3.2	33
34	Lattice dynamics and electron-phonon coupling in the $\text{BEDT-TTF} \cdot \text{I}_3$ organic superconductor. <i>Physical Review B</i> , 2000, 62, 14476-14486.	3.2	33
35	Exploring the polymorphism of crystalline pentacene. <i>Organic Electronics</i> , 2004, 5, 1-6.	2.6	33
36	Molecular Dynamics Simulations for a Pentacene Monolayer on Amorphous Silica. <i>ChemPhysChem</i> , 2009, 10, 1783-1788.	2.1	32

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37	Pressure and temperature effects in lattice dynamics: the case of naphthalene. <i>Chemical Physics</i> , 1995, 198, 79-89.	1.9	31
38	A spectroscopic investigation of the temperature and solvent sensitivities of resorufin. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1989, 85, 1935.	1.1	30
39	BEDT-TTF organic superconductors: The role of phonons. <i>Physical Review B</i> , 2002, 66, .	3.2	30
40	Two New Polymorphs of the Organic Semiconductor 9,10-Diphenylanthracene: Raman and X-ray Analysis. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1831-1840.	3.1	29
41	Micro Raman Investigation of the Photodimerization Reaction of 9-Cyanoanthracene in the Solid State. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9628-9635.	3.1	27
42	A scaling approximation for structure factors in the integral equation theory of polydisperse nonionic colloidal fluids. <i>Journal of Chemical Physics</i> , 1999, 111, 7636-7645.	3.0	26
43	Polymorphs of $\hat{1}\pm$ -sexithiophene probed by lattice phonon Raman microscopy. <i>Chemical Physics</i> , 2006, 328, 125-131.	1.9	26
44	Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4380-4390.	5.3	26
45	Absorption, Photoluminescence, and Polarized Raman Spectra of a Fourfold Alkoxy-Substituted Phthalocyanine Liquid Crystal. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12150-12157.	3.1	25
46	Direct evidence of overdamped Peierls-coupled modes in the temperature-induced phase transition in tetrathiafulvalene-chloranil. <i>Physical Review B</i> , 2008, 78, .	3.2	24
47	Vibration-Rotation Spectra of $^{13}\text{C}$ -Containing Acetylene: The $\hat{1}\frac{1}{2}1/\hat{1}\frac{1}{2} + 2\hat{1}\frac{1}{2}5$ Fermi Dyad. <i>Journal of Molecular Spectroscopy</i> , 1994, 164, 219-232.	1.2	23
48	Organic Semiconductors: Polymorphism, Phonon Dynamics and Carrier-Phonon Coupling in Pentacene. <i>Molecular Crystals and Liquid Crystals</i> , 2004, 416, 145-154.	0.9	23
49	Inherent Structures of Crystalline Tetracene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10858-10862.	2.5	22
50	Structural, Spectroscopic, and Computational Characterization of the Concomitant Polymorphs of the Natural Semiconductor Indigo. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18422-18431.	3.1	22
51	Pressure-induced phase transitions in 9,10-anthracene derivatives: anthraquinone. <i>Chemical Physics</i> , 1995, 191, 177-184.	1.9	21
52	Spectroscopic and Structural Characterization of Two Polymorphs of 1,1,4,4-Tetraphenyl-1,3-butadiene. <i>Crystal Growth and Design</i> , 2010, 10, 2752-2758.	3.0	21
53	Tuning polymorphism in 2,3-thienoimide capped oligothiophene based field-effect transistors by implementing vacuum and solution deposition methods. <i>Journal of Materials Chemistry C</i> , 2018, 6, 5601-5608.	5.5	21
54	Lattice dynamics of TTF $\hat{1}\hat{1}$ CA across the neutral $\hat{1}\hat{1}$ ionic transition. <i>Chemical Physics</i> , 2006, 325, 71-77.	1.9	20

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55	Polymorphism and Phonon Dynamics of $\beta$ -Quaterthiophene. <i>ChemPhysChem</i> , 2009, 10, 657-663.	2.1	20
56	PENTACENE AT HIGH PRESSURE. <i>High Pressure Research</i> , 2003, 23, 349-354.	1.2	19
57	Crystal-to-Crystal Photoinduced Reaction of Dinitroanthracene to Anthraquinone. <i>Journal of the American Chemical Society</i> , 2012, 134, 17671-17679.	13.7	19
58	Phonon dynamics and electron-phonon coupling in pristine picene. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1694-1699.	2.8	19
59	An Alternative Strategy to Polymorph Recognition at Work: The Emblematic Case of Coronene. <i>Crystal Growth and Design</i> , 2018, 18, 4869-4873.	3.0	19
60	Fast identification of rubrene polymorphs by lattice phonon Raman microscopy. <i>Solid State Sciences</i> , 2017, 71, 146-151.	3.2	18
61	High-Pressure Dissociation of Crystalline para-Diiodobenzene: $\omega$ Optical Experiments and Car-Parrinello Calculations. <i>Journal of the American Chemical Society</i> , 2005, 127, 3038-3043.	13.7	16
62	Are Crystal Polymorphs Predictable? The Case of Sexithiophene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6715-6722.	2.5	16
63	A molecular dynamics simulation of crystalline S8. <i>Chemical Physics</i> , 1992, 165, 313-322.	1.9	15
64	Vibration-rotation spectra of $^{13}\text{C}$ containing acetylene: anharmonic resonances. <i>Chemical Physics</i> , 1995, 190, 279-290.	1.9	15
65	Stark and Frequency Measurements in the FIR Spectrum of $\text{H}_2\text{O}_2$ . <i>Journal of Molecular Spectroscopy</i> , 1996, 177, 115-123.	1.2	15
66	Organic metal-organic semiconductor blended contacts in single crystal field-effect transistors. <i>Journal of Materials Chemistry</i> , 2012, 22, 16011.	6.7	14
67	Crystal Structure of the 9-Anthracene-Carboxylic Acid Photochemical Dimer and Its Solvates by X-ray Diffraction and Raman Microscopy. <i>Crystal Growth and Design</i> , 2017, 17, 3361-3370.	3.0	14
68	Spectroscopic identification of quinacridone polymorphs for organic electronics. <i>CrystEngComm</i> , 2019, 21, 3702-3708.	2.6	13
69	Phase recognition by lattice phonon Raman spectra: The triclinic structure of the organic semiconductor dibenzo-tetrathiafulvalene. <i>Chemical Physics Letters</i> , 2012, 523, 74-77.	2.6	12
70	Raman investigation of polymorphism in 1,1,4,4-tetraphenylbutadiene. <i>Journal of Raman Spectroscopy</i> , 2013, 44, 905-908.	2.5	11
71	Solid-state photodimerization of 9-methyl-anthracene. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 271-277.	2.5	11
72	Do Computed Crystal Structures of Nonpolar Molecules Depend on the Electrostatic Interactions? The Case of Tetracene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1085-1089.	2.5	10

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73	A synergic approach of X-ray powder diffraction and Raman spectroscopy for crystal structure determination of 2,3-thienoimide capped oligothiophenes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3630-3636.	2.8	10
74	Bulk and Surface-Stabilized Structures of Paracetamol Revisited by Raman Confocal Microscopy. <i>ACS Omega</i> , 2018, 3, 9564-9571.	3.5	10
75	Lattice dynamics and electron-phonon coupling in pentacene crystal structures. <i>Macromolecular Symposia</i> , 2004, 212, 375-380.	0.7	9
76	Exploration of the polymorph landscape for 1,1,4,4-tetraphenyl-1,3-butadiene. <i>CrystEngComm</i> , 2014, 16, 8205-8213.	2.6	9
77	Crystal alignment of surface stabilized polymorph in thioindigo films. <i>Dyes and Pigments</i> , 2020, 172, 107847.	3.7	9
78	Substrate-Induced Phase of a Benzothiophene Derivative Detected by Mid-Infrared and Lattice Phonon Raman Spectroscopy. <i>ChemPhysChem</i> , 2018, 19, 993-1000.	2.1	8
79	Calculation of Duschinsky effect in phenol. <i>Journal of Molecular Structure</i> , 1992, 266, 235-239.	3.6	7
80	Vibration-Rotation Spectra of <sup>13</sup> C-Containing Acetylene: The Stretching Fundamentals. <i>Journal of Molecular Spectroscopy</i> , 1995, 169, 148-153.	1.2	7
81	Temperature evolution of pentacene crystal structure and phonon dynamics. <i>Materials Research Society Symposia Proceedings</i> , 2002, 725, 1.	0.1	7
82	Electrochemical Approach for the Production of Layered Double Hydroxides with a Well-Defined Co/Me <sup>III</sup> Ratio. <i>Chemistry - A European Journal</i> , 2019, 25, 16301-16310.	3.3	7
83	Solution equilibrium between two structures of Perylene-F2TCNQ charge transfer co-crystals. <i>Journal of Crystal Growth</i> , 2019, 516, 45-50.	1.5	7
84	Precursor polymorph determines the organic semiconductor structure formed upon annealing. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10865-10874.	5.5	7
85	The effect of pressure on the photodimerization of 7-methoxycoumarin crystal. <i>Chemical Physics Letters</i> , 1994, 218, 568-573.	2.6	6
86	Electron-phonon coupling in BEDT-TTF (ET) superconductors. <i>Synthetic Metals</i> , 2000, 109, 13-17.	3.9	6
87	DFT Investigation of Oligothiophenes on a Si(001) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20068-20075.	3.1	6
88	Photoluminescence as a probe of molecular organization in PDI8-CN2 ultra-thin films. <i>Journal of Luminescence</i> , 2017, 187, 403-409.	3.1	6
89	Growth, morphology and molecular orientation of controlled Indigo thin films on silica surfaces. <i>Surfaces and Interfaces</i> , 2021, 24, 101058.	3.0	6
90	Molecular anharmonicity: A computer-aided treatment. <i>Journal of Computational Chemistry</i> , 1999, 20, 1716-1730.	3.3	5

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91	Coupling between intramolecular and lattice vibrations in solid para-diiodobenzene. <i>Chemical Physics Letters</i> , 2000, 325, 599-604.	2.6	5
92	Coupling between lattice and intramolecular modes in 9,10-dimethylantracene: Raman spectra under pressure and quasi-harmonic lattice dynamics calculations. <i>Chemical Physics</i> , 2001, 273, 197-206.	1.9	5
93	Surface Induced Phenytoin Polymorph. 1. Full Structure Solution by Combining Grazing Incidence X-ray Diffraction and Crystal Structure Prediction. <i>Crystal Growth and Design</i> , 2019, 19, 6058-6066.	3.0	5
94	Experimental Estimate of the Holstein Electron-Phonon Coupling Constants in Perylene. <i>Advanced Electronic Materials</i> , 2020, 6, 2000208.	5.1	5
95	Electrosynthesis and characterization of Layered Double Hydroxides on different supports. <i>Applied Clay Science</i> , 2021, 202, 105949.	5.2	5
96	The impact of solid solution composition on kinetics and mechanism of [2 + 2] photodimerization of cinnamic acid derivatives. <i>CrystEngComm</i> , 2021, 23, 1352-1359.	2.6	5
97	Theoretical studies on the two-photon vibronic spectra of azines: Pyridine, pyrazine and pyrimidine. <i>Chemical Physics</i> , 1988, 125, 1-9.	1.9	4
98	An intra-molecular potential for S8. <i>Journal of Molecular Structure</i> , 1992, 266, 229-234.	3.6	4
99	Temperature dependence of structure and phonons of $\hat{1}\pm$ - and $\hat{1}^2$ -TTF crystals. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 4170-4175.	2.8	4
100	(Perylene)3-(TCNQF1)2: Yet Another Member in the Series of Perylene-TCNQx Polymorphic Charge Transfer Crystals. <i>Crystals</i> , 2020, 10, 177.	2.2	4
101	Intermolecular phonons in BEDT-TTF crystals. <i>Synthetic Metals</i> , 1997, 85, 1561-1562.	3.9	3
102	In Search of Surface-Induced Crystal Structures: The Case of Tyrian Purple. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17702-17710.	3.1	3
103	Visualizing a SCSC [2 + 2] photodimerization through its lattice dynamics: an experimental and theoretical investigation. <i>ChemPhysChem</i> , 2022, , .	2.1	3
104	Simulated Raman spectra of four tetraphenylbutadiene polymorphs. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25503.	2.0	2
105	Bulk and Surface-Mediated Polymorphs of Bio-Inspired Dyes Organic Semiconductors: The Role of Lattice Phonons in their Investigation. <i>Israel Journal of Chemistry</i> , 0, , .	2.3	2
106	Raman phonon spectra and lattice dynamics of 7-methoxycoumarin under pressure. <i>Chemical Physics Letters</i> , 1995, 246, 619-625.	2.6	1
107	High-Pressure Raman Spectra of p-Diiodobenzene. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11070-11074.	2.5	1
108	Surface Induced Phenytoin Polymorph. 2. Structure Validation by Comparing Experimental and Density Functional Theory Raman Spectra. <i>Crystal Growth and Design</i> , 2019, 19, 6067-6073.	3.0	1

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109	Epitaxial relation of carbamazepine and its precursor template extracted from rotating grazing incidence X-ray diffraction. <i>Thin Solid Films</i> , 2019, 683, 67-73.	1.8	1
110	Engineering Plastic Phase Transitions via Solid Solutions: The Case of "Reordering Frustration" in Ionic Plastic Crystals of Hydroxyquinuclidinium Salts. <i>Molecular Systems Design and Engineering</i> , 0, , .	3.4	1
111	Vibronic activity in the two-photon spectrum of pyrimidine. <i>Journal of Molecular Structure</i> , 1988, 175, 153-158.	3.6	0
112	Solvation dynamics in methanol and n-butanol. Comparison between temperature-dependent fluorescence and dielectric data. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1988, 84, 1747.	1.1	0
113	The Effect of Pressure on Vibrational Spectra of the Chiral Coordination Compound Ni[(R,R)bdtp] <sub>2</sub> . <i>High Pressure Research</i> , 2002, 22, 99-103.	1.2	0
114	Organic superconductors: How can we increase the critical temperature?. <i>Synthetic Metals</i> , 2003, 137, 1273-1274.	3.9	0