Raffaele Guido Della Valle

List of Publications by Year
in descending order

141 papers	4,454 citations	126708 33 h-index	118652 62 g-index
142 all docs	142 docs citations	142 times ranked	4074 citing authors

#	Article	IF	Citations
1	A third blind test of crystal structure prediction. Acta Crystallographica Section B: Structural Science, 2005, 61, 511-527.	1.8	373
2	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
3	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
4	The oxidation of tyrosine and tryptophan studied by a molecular dynamics normal hydrogen electrode. Journal of Chemical Physics, 2011, 134, 244508.	1.2	115
5	Peierls and Holstein carrier-phonon coupling in crystalline rubrene. Physical Review B, 2010, 82, .	1.1	113
6	Glycerol condensed phases Part I. A molecular dynamics study. Physical Chemistry Chemical Physics, 1999, 1, 871-877.	1.3	112
7	Molecular dynamics simulation of silica liquid and glass. Journal of Chemical Physics, 1992, 97, 2682-2689.	1.2	108
8	Epitaxial Growth of Ï€-Stacked Perfluoropentacene on Graphene-Coated Quartz. ACS Nano, 2012, 6, 10874-10883.	7.3	108
9	Probing polymorphs of organic semiconductors by lattice phonon Raman microscopy. CrystEngComm, 2008, 10, 937.	1.3	103
10	Structure, Stoichiometry, and Charge Transfer in Cocrystals of Perylene with TCNQ-F_x. Crystal Growth and Design, 2016, 16, 3028-3036.	1.4	99
11	High-pressure densification of silica glass: A molecular-dynamics simulation. Physical Review B, 1996, 54, 3809-3816.	1.1	78
12	Anharmonic processes in molecular crystals. Calculation of the anharmonic shifts, bandwidths and energy decay processes in crystalline naphthalene. Chemical Physics, 1983, 74, 179-195.	0.9	77
13	Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene. ChemPhysChem, 2009, 10, 2265-2273.	1.0	77
14	Phonons and structures of tetracene polymorphs at low temperature and high pressure. Physical Review B, 2004, 70, .	1.1	75
15	Characterization of Phase Purity in Organic Semiconductors by Lattice-Phonon Confocal Raman Mapping: Application to Pentacene. Advanced Materials, 2005, 17, 2549-2553.	11.1	67
16	Local-mode to normal-mode hamiltonian transformation forX-H stretchings. Molecular Physics, 1988, 63, 611-621.	0.8	62
17	Inherent structures of crystalline pentacene. Journal of Chemical Physics, 2003, 118, 807-815.	1.2	62
18	The four polymorphic modifications of the semiconductor dibenzo-tetrathiafulvalene. CrystEngComm, 2008, 10, 1899.	1.3	62

#	Article	IF	Citations
19	Predicting the Anchoring of Liquid Crystals at a Solid Surface: 5-Cyanobiphenyl on Cristobalite and Glassy Silica Surfaces of Increasing Roughness. Langmuir, 2013, 29, 8950-8958.	1.6	62
20	High dimensional anharmonic potential energy surfaces: The case of methane. Journal of Chemical Physics, 1999, 110, 7339-7347.	1.2	58
21	Probing Pentacene Polymorphs by Lattice Dynamics Calculations. Journal of the American Chemical Society, 2002, 124, 2128-2129.	6.6	57
22	Crystal structure of oligoacenes under high pressure. Physical Review B, 2006, 74, .	1.1	56
23	Pressure-induced phase transition in pentacene. Chemical Physics Letters, 2003, 375, 490-494.	1.2	55
24	Intramolecular and Low-Frequency Intermolecular Vibrations of Pentacene Polymorphs as a Function of Temperature. Journal of Physical Chemistry B, 2004, 108, 1822-1826.	1.2	53
25	Structure and Morphology of PDI8â€CN2 for nâ€Type Thinâ€Film Transistors. Advanced Functional Materials, 2012, 22, 943-953.	7.8	50
26	Polarized Raman Spectra of a Rubrene Single Crystal. Journal of Physical Chemistry C, 2008, 112, 17416-17422.	1.5	45
27	Interaction of charge carriers with lattice and molecular phonons in crystalline pentacene. Journal of Chemical Physics, 2011, 135, 084701.	1.2	44
28	DFT-Assisted Polymorph Identification from Lattice Raman Fingerprinting. Journal of Physical Chemistry Letters, 2017, 8, 3690-3695.	2.1	42
29	Test of a pairwise additive ionic potential model for silica. Journal of Chemical Physics, 1991, 94, 5056-5060.	1.2	40
30	A molecular dynamics study of the vibrational properties of silica glass. Chemical Physics, 1994, 179, 411-419.	0.9	40
31	Structure and dynamics of pentacene on SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: From monolayer to bulk structure. Physical Review B, 2012, 85, .	1.1	40
32	MD Simulation of the Na+â^'Phenylalanine Complex in Water:Â Competition between Cationâ^'Ï€ Interaction and Aqueous Solvation. Journal of Physical Chemistry B, 2005, 109, 23016-23023.	1.2	34
33	Quasi harmonic lattice dynamics: the phase diagram of benzene. Chemical Physics, 1996, 202, 231-241.	0.9	33
34	Quasiharmonic lattice-dynamics and molecular-dynamics calculations for the Lennard-Jones solids. Physical Review B, 1998, 58, 206-212.	1.1	33
35	Lattice dynamics and electron-phonon coupling in theÎ²â^'(BEDTâ^'TTF)2I3organic superconductor. Physical Review B, 2000, 62, 14476-14486.	1.1	33
36	Exploring the polymorphism of crystalline pentacene. Organic Electronics, 2004, 5, 1-6.	1.4	33

#	Article	IF	Citations
37	Molecular Dynamics Simulations for a Pentacene Monolayer on Amorphous Silica. ChemPhysChem, 2009, 10, 1783-1788.	1.0	32
38	Pressure and temperature effects in lattice dynamics: the case of naphthalene. Chemical Physics, 1995, 198, 79-89.	0.9	31
39	BEDT-TTF organic superconductors: The role of phonons. Physical Review B, 2002, 66, .	1.1	30
40	Two New Polymorphs of the Organic Semiconductor 9,10-Diphenylanthracene: Raman and X-ray Analysis. Journal of Physical Chemistry C, 2016, 120, 1831-1840.	1.5	29
41	Towards an effective potential for the monomer, dimer, hexamer, solid, and liquid forms of hydrogen fluoride. Physical Review B, 1999, 59, 13699-13706.	1.1	28
42	NH2 inversion potential in the S0 and S1 electronic states of aniline: fit to the (ro-)vibrational data and comparison with ab initio and density functional results. Chemical Physics Letters, 2000, 327, 45-53.	1.2	27
43	Micro Raman Investigation of the Photodimerization Reaction of 9-Cyanoanthracene in the Solid State. Journal of Physical Chemistry C, 2014, 118, 9628-9635.	1.5	27
44	A scaling approximation for structure factors in the integral equation theory of polydisperse nonionic colloidal fluids. Journal of Chemical Physics, 1999, 111, 7636-7645.	1.2	26
45	Polymorphs of Î±-sexithiophene probed by lattice phonon Raman microscopy. Chemical Physics, 2006, 328, 125-131.	0.9	26
46	Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. Journal of Chemical Theory and Computation, 2018, 14, 4380-4390.	2.3	26
47	Absorption, Photoluminescence, and Polarized Raman Spectra of a Fourfold Alkoxy-Substituted Phthalocyanine Liquid Crystal. Journal of Physical Chemistry C, 2011, 115, 12150-12157.	1.5	25
48	Energy decay mechanisms and anharmonic lattice dynamics: The case of solid nitrogen. Chemical Physics, 1985, 100, 315-329.	0.9	24
49	Direct evidence of overdamped Peierls-coupled modes in the temperature-induced phase transition in tetrathiafulvalene-chloranil. Physical Review B, 2008, 78, .	1.1	24
50	Electrostatic Interactions Shape Molecular Organization and Electronic Structure of Organic Semiconductor Blends. Chemistry of Materials, 2020, 32, 1261-1271.	3.2	24
51	Phonon dispersion curves and phonon lifetimes in crystalline ammonia. Chemical Physics, 1979, 44, 189-196.	0.9	23
52	Molecular dynamics simulation of crystalline naphthalene. Acta Crystallographica Section A: Foundations and Advances, 1984, 40, 297-305.	0.3	23
53	Organic Semiconductors: Polymorphism, Phonon Dynamics and Carrier-Phonon Coupling in Pentacene. Molecular Crystals and Liquid Crystals, 2004, 416, 145-154.	0.4	23
54	Lattice dynamics of solid Î±-carbon monoxide. Chemical Physics, 1985, 96, 361-369.	0.9	22

#	Article	IF	Citations
55	An improved representation for the highâ€density structure of Lennardâ€Jones systems: From liquid toward glass. Journal of Chemical Physics, 1993, 99, 6915-6922.	1.2	22
56	Inherent Structures of Crystalline Tetracene. Journal of Physical Chemistry A, 2006, 110, 10858-10862.	1.1	22
57	Structural, Spectroscopic, and Computational Characterization of the Concomitant Polymorphs of the Natural Semiconductor Indigo. Journal of Physical Chemistry C, 2018, 122, 18422-18431.	1.5	22
58	Singlet exciton fission via an intermolecular charge transfer state in coevaporated pentacene-perfluoropentacene thin films. Journal of Chemical Physics, 2019, 151, 164706.	1.2	22
59	Pressure-induced phase transitions in 9,10-anthracene derivatives: anthraquinone. Chemical Physics, 1995, 191, 177-184.	0.9	21
60	Spectroscopic and Structural Characterization of Two Polymorphs of 1,1,4,4-Tetraphenyl-1,3-butadiene. Crystal Growth and Design, 2010, 10, 2752-2758.	1.4	21
61	Lattice dynamics of TTFâ€“CA across the neutralâ€“ionic transition. Chemical Physics, 2006, 325, 71-77.	0.9	20
62	Polymorphism and Phonon Dynamics of Î±â€Quaterthiophene. ChemPhysChem, 2009, 10, 657-663.	1.0	20
63	PENTACENE AT HIGH PRESSURE. High Pressure Research, 2003, 23, 349-354.	0.4	19
64	Carâ€'Parrinello MD Simulations for the Na⁺â€'Phenylalanine Complex in Aqueous Solution. Journal of Physical Chemistry B, 2008, 112, 12783-12789.	1.2	19
65	Crystal-to-Crystal Photoinduced Reaction of Dinitroanthracene to Anthraquinone. Journal of the American Chemical Society, 2012, 134, 17671-17679.	6.6	19
66	Phonon dynamics and electronâ€“phonon coupling in pristine picene. Physical Chemistry Chemical Physics, 2012, 14, 1694-1699.	1.3	19
67	An Alternative Strategy to Polymorph Recognition at Work: The Emblematic Case of Coronene. Crystal Growth and Design, 2018, 18, 4869-4873.	1.4	19
68	Fast identification of rubrene polymorphs by lattice phonon Raman microscopy. Solid State Sciences, 2017, 71, 146-151.	1.5	18
69	Vibrational analysis of the carbon-hydrogen stretching overtones in pyridine and 2,6-lutidine. The Journal of Physical Chemistry, 1991, 95, 3027-3031.	2.9	17
70	Microstructural analysis of simulatedNi33Y67glass. Physical Review B, 1994, 49, 12625-12632.	1.1	17
71	High-Pressure Dissociation of Crystallinepara-Diiodobenzene:Â Optical Experiments and Carâ€'Parrinello Calculations. Journal of the American Chemical Society, 2005, 127, 3038-3043.	6.6	16
72	Are Crystal Polymorphs Predictable? The Case of Sexithiophene. Journal of Physical Chemistry A, 2008, 112, 6715-6722.	1.1	16

#	Article	IF	Citations
73	Rotational spectra of several vibrational excited states of axial and equatorial cyanocyclobutane and potential energy function of the ring puckering. Journal of Molecular Spectroscopy, 1988, 129, 284-292.	0.4	15
74	Effect of pressure on lattice modes and electronic excitations of 9,10-diiodoanthracene crystals. Journal of Chemical Physics, 1997, 107, 4628-4634.	1.2	14
75	Ab initiomolecular dynamics study of ascorbic acid in aqueous solution. Molecular Physics, 2007, 105, 17-23.	0.8	14
76	Crystal Structure of the 9-Anthraceneâ€“Carboxylic Acid Photochemical Dimer and Its Solvates by X-ray Diffraction and Raman Microscopy. Crystal Growth and Design, 2017, 17, 3361-3370.	1.4	14
77	Equation of motion for the Greenâ€™s function in anharmonic solids. Physical Review B, 1992, 46, 6141-6149.	1.1	13
78	First Principles Study of Alkaliâ^'Tyrosine Complexes: Alkali Solvation and Redox Properties. Journal of Chemical Theory and Computation, 2008, 4, 1049-1056.	2.3	13
79	Phase recognition by lattice phonon Raman spectra: The triclinic structure of the organic semiconductor dibenzo-tetrathiafulvalene. Chemical Physics Letters, 2012, 523, 74-77.	1.2	12
80	Anharmonic interactions in molecular crystals. Two-phonon absorption in crystalline OCS. Chemical Physics, 1979, 43, 385-393.	0.9	11
81	Raman investigation of polymorphism in 1,1,4,4â€tetraphenylâ€butadiene. Journal of Raman Spectroscopy, 2013, 44, 905-908.	1.2	11
82	Solid-state photodimerization of 9-methyl-anthracene. Journal of Raman Spectroscopy, 2017, 48, 271-277.	1.2	11
83	Efficient calculation of high-order self-energy corrections to phonon linewidths: Application to Î±-nitrogen. Physical Review B, 1993, 47, 11124-11133.	1.1	10
84	Do Computed Crystal Structures of Nonpolar Molecules Depend on the Electrostatic Interactions? The Case of Tetracene. Journal of Physical Chemistry A, 2008, 112, 1085-1089.	1.1	10
85	A synergic approach of X-ray powder diffraction and Raman spectroscopy for crystal structure determination of 2,3-thienoimide capped oligothiophenes. Physical Chemistry Chemical Physics, 2018, 20, 3630-3636.	1.3	10
86	Bulk and Surface-Stabilized Structures of Paracetamol Revisited by Raman Confocal Microscopy. ACS Omega, 2018, 3, 9564-9571.	1.6	10
87	Non-additive Lennard-Jones model for the structure of Ni33Y67 metallic glass: integral equation and molecular dynamics calculations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1993, 165, 183-187.	2.6	9
88	Lattice dynamics and electron-phonon coupling in pentacene crystal structures. Macromolecular Symposia, 2004, 212, 375-380.	0.4	9
89	Exploration of the polymorph landscape for 1,1,4,4-tetraphenyl-1,3-butadiene. CrystEngComm, 2014, 16, 8205-8213.	1.3	9
90	Potential models and torsional stability in molecular crystals. Chemical Physics Letters, 1984, 104, 435-439.	1.2	8

#	Article	IF	Citations
91	Recursive computation of many-phonon densities of states. Physical Review Letters, 1987, 59, 2196-2198.	2.9	8
92	Linewidth of the 991 cmâ˜'1 mode in benzene at high pressures. Chemical Physics Letters, 1988, 148, 45-51.	1.2	8
93	Lattice phonons in neutral BEDT-TTF crystal. Chemical Physics Letters, 1997, 274, 478-484.	1.2	8
94	High pressure Raman spectra and pressureâ€induced phase transitions of Î²â€9,10â€dichloroanthracene. Journal of Chemical Physics, 1988, 89, 3163-3167.	1.2	7
95	Structure and phonons of Î±-(ET)2+I3â˜' crystals. Physica B: Condensed Matter, 1999, 265, 195-198.	1.3	7
96	Temperature evolution of pentacene crystal structure and phonon dynamics. Materials Research Society Symposia Proceedings, 2002, 725, 1.	0.1	7
97	Local mode and normal mode models for molecules with two non-equivalent Câ€“H bonds. Molecular Physics, 2007, 105, 1779-1787.	0.8	7
98	Solution equilibrium between two structures of Perylene-F2TCNQ charge transfer co-crystals. Journal of Crystal Growth, 2019, 516, 45-50.	0.7	7
99	Precursor polymorph determines the organic semiconductor structure formed upon annealing. Journal of Materials Chemistry C, 2021, 9, 10865-10874.	2.7	7
100	A dynamical model of excimer instability in molecular crystals. Chemical Physics, 1987, 116, 141-149.	0.9	6
101	Molecular-dynamics simulation of glassyCu33Y67. Physical Review B, 1994, 50, 3620-3624.	1.1	6
102	The effect of pressure on the photodimerization of 7-methoxycoumarin crystal. Chemical Physics Letters, 1994, 218, 568-573.	1.2	6
103	Pressure-induced phase transitions in quasi-one-dimensional anthracene derivatives. Physica B: Condensed Matter, 1999, 265, 199-202.	1.3	6
104	Electronâ€“phonon coupling in BEDT-TTF (ET) superconductors. Synthetic Metals, 2000, 109, 13-17.	2.1	6
105	DFT Investigation of Oligothiophenes on a Si(001) Surface. Journal of Physical Chemistry C, 2010, 114, 20068-20075.	1.5	6
106	The Chemistry of Niâ€“Sb Carbonyl Clusters â€“ Synthesis and Characterization of the [Ni₁₉Sb₄(CO)₂₆]^{4â€“} Tetraanion and the Viologen Salts of [Ni₁₃Sb₂(CO)₂₄]^{nâ€“} Carbonyl Clusters. European Journal of Inorganic Chemistry, 2014, 2014, 4151-4158.	1.0	6
107	Photoluminescence as a probe of molecular organization in PDI8-CN2 ultra-thin films. Journal of Luminescence, 2017, 187, 403-409.	1.5	6
108	Growth, morphology and molecular orientation of controlled Indigo thin films on silica surfaces. Surfaces and Interfaces, 2021, 24, 101058.	1.5	6

#	Article	IF	Citations
109	Theoretical analysis of resonant raman scattering: Simulations of lineshapes and excitation profiles. Chemical Physics, 1985, 94, 351-364.	0.9	5
110	Vibrational density of states and homogeneous linewidth in molecular crystals: Many-phonon processes in nitrogen. Physical Review B, 1997, 55, 14855-14864.	1.1	5
111	Molecular anharmonicity: A computer-aided treatment. Journal of Computational Chemistry, 1999, 20, 1716-1730.	1.5	5
112	Coupling between intramolecular and lattice vibrations in solid para-diiodobenzene. Chemical Physics Letters, 2000, 325, 599-604.	1.2	5
113	Coupling between lattice and intramolecular modes in 9,10-dimethylanthracene: Raman spectra under pressure and quasi-harmonic lattice dynamics calculations. Chemical Physics, 2001, 273, 197-206.	0.9	5
114	Surface Induced Phenytoin Polymorph. 1. Full Structure Solution by Combining Grazing Incidence X-ray Diffraction and Crystal Structure Prediction. Crystal Growth and Design, 2019, 19, 6058-6066.	1.4	5
115	Experimental Estimate of the Holstein Electronâ€“Phonon Coupling Constants in Perylene. Advanced Electronic Materials, 2020, 6, 2000208.	2.6	5
116	The impact of solid solution composition on kinetics and mechanism of [2 + 2] photodimerization of cinnamic acid derivatives. CrystEngComm, 2021, 23, 1352-1359.	1.3	5
117	Effects of dampings and dephasings in resonance raman spectroscopy. Chemical Physics Letters, 1985, 115, 428-433.	1.2	4
118	The effect of pressure on the electronic spectra of anthracene derivatives. Journal of Luminescence, 1987, 38, 311-313.	1.5	4
119	Stability under pressure of excimers of anthracene derivatives. Journal of Luminescence, 1992, 53, 110-112.	1.5	4
120	Temperature dependence of structure and phonons of Î±- and Î²-TTF crystals. Physical Chemistry Chemical Physics, 2001, 3, 4170-4175.	1.3	4
121	(Perylene)3-(TCNQF1)2: Yet Another Member in the Series of Peryleneâ€“TCNQFx Polymorphic Charge Transfer Crystals. Crystals, 2020, 10, 177.	1.0	4
122	Lattice dynamics of ionic molecular crystals in the rigid ion approximation, phases II and III of sodium superoxide. Canadian Journal of Physics, 1984, 62, 54-64.	0.4	3
123	Non-perturbative theory of four-wave light scattering in strong fields. Chemical Physics, 1987, 115, 169-186.	0.9	3
124	In Search of Surface-Induced Crystal Structures: The Case of Tyrian Purple. Journal of Physical Chemistry C, 2020, 124, 17702-17710.	1.5	3
125	Visualizing a SCSC [2 + 2] photodimerization through its lattice dynamics: an experimental and theoretical investigation. ChemPhysChem, 2022, , .	1.0	3
126	Polar modes in molecular crystals: Ewald splitting of infrared and Raman lines. Canadian Journal of Physics, 1984, 62, 1237-1247.	0.4	2

#	Article	IF	Citations
127	Simulated Raman spectra of four tetraphenylbutadiene polymorphs. International Journal of Quantum Chemistry, 2018, 118, e25503.	1.0	2
128	Transient behaviour of coherent and incoherent processes in a three-level system. Chemical Physics, 1986, 103, 287-294.	0.9	1
129	Lattice dynamics of YBa 2 Cu 3 O 6 and YBa 2 Cu 3 O 7 , a rigid ion model. Physica C: Superconductivity and Its Applications, 1989, 162-164, 1429-1430.	0.6	1
130	Raman phonon spectra and lattice dynamics of 7-methoxycoumarin under pressure. Chemical Physics Letters, 1995, 246, 619-625.	1.2	1
131	Raman phonon spectra and lattice dynamics of 9,10-dinitroanthracene under pressure. High Pressure Research, 2000, 18, 233-238.	0.4	1
132	Computer-Aided Series Expansion for Phonon Self-Energy. Journal of Computational Physics, 2000, 165, 428-436.	1.9	1
133	Pressure and temperature effects in lattice dynamics: 1,4-dibromonaphthalene. Chemical Physics, 2000, 262, 437-444.	0.9	1
134	High-Pressure Raman Spectra ofp-Diiodobenzene. Journal of Physical Chemistry A, 2000, 104, 11070-11074.	1.1	1
135	Surface Induced Phenytoin Polymorph. 2. Structure Validation by Comparing Experimental and Density Functional Theory Raman Spectra. Crystal Growth and Design, 2019, 19, 6067-6073.	1.4	1
136	Non perturbative theory of electronic resonant coherent Raman scattering (CARS, CSRS). Journal of Molecular Structure, 1986, 142, 489-492.	1.8	0
137	Lattice stability of YBa2Cu3O6 and YBa2Cu3O7. Physica C: Superconductivity and Its Applications, 1991, 185-189, 1679-1680.	0.6	0
138	Lattice dynamics and e-ph coupling in BEDT-TTF superconductors. Synthetic Metals, 1999, 103, 2083.	2.1	0
139	Organic superconductors: How can we increase the critical temperature?. Synthetic Metals, 2003, 137, 1273-1274.	2.1	0
140	Inside Cover: Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene (ChemPhysChem 13/2009). ChemPhysChem, 2009, 10, 2158-2158.	1.0	0
141	Electron-Intermolecular Phonon Coupling in Î²-Phase BEDT-TTF Organic Superconductors. , 2002, , 251-254.		0