anna Painelli

List of Publications by Citations

171 papers	3,942 citations	36 h-index	55 g-index
187 ext. papers	4,297 ext. citations	4.8 avg, IF	5.39 L-index

#	Paper	IF	Citations
171	Charge instability in quadrupolar chromophores: symmetry breaking and solvatochromism. *Journal of the American Chemical Society*, **2006**, 128, 15742-55	16.4	330
170	Electron□molecular vibration (e□hν) coupling in charge-transfer compounds and its consequences on the optical spectra: A theoretical framework. *Journal of Chemical Physics*, **1986**, 84, 5655-5671	3.9	181
169	Polar Dyes in Solution: A Joint Experimental and Theoretical Study of Absorption and Emission Band Shapes. *Journal of Physical Chemistry A*, **2002**, 106, 6286-6294	2.8	114
168	Vibronic contribution to static NLO properties: exact results for the DA dimer. *Chemical Physics Letters*, **1998**, 285, 352-358	2.5	97
167	Essential-State Model for Polymethine Dyes: Symmetry Breaking and Optical Spectra. *Journal of Physical Chemistry Letters*, **2010**, 1, 1800-1804	6.4	80
166	Symmetry breaking in octupolar chromophores: solvatochromism and electroabsorption. *Journal of Physical Chemistry B*, **2008**, 112, 5079-87	3.4	80
165	Optical Spectra of Push□Pull Chromophores in Solution:□A Simple Model. *Journal of Physical Chemistry A*, **2000**, 104, 11041-11048	2.8	75
164	Zero-temperature phase diagram of mixed-stack charge-transfer crystals. *Physical Review B*, **1988**, 37, 5748-5760	3.3	75
163	Amplification of NLO responses: vibronic and solvent effects in push□pull polyenes. *Chemical Physics*, **1999**, 245, 185-197	2.3	70
162	Multichromophores for nonlinear optics: designing the material properties by electrostatic interactions. *ChemPhysChem*, **2007**, 8, 2433-44	3.2	69
161	Chiral interactions in azobenzene dimers: a combined experimental and theoretical study. *Chemistry - A European Journal*, **2005**, 11, 6053-63	4.8	69
160	A non-perturbative approach to solvatochromic shifts of push□pull chromophores. *Chemical Physics Letters*, **1999**, 312, 211-220	2.5	69
159	Supramolecular interactions in clusters of polar and polarizable molecules. *Physical Review B*, **2003**, 68,	3.3	63
158	Regular-dimerized stack and neutral-ionic interfaces in mixed-stack organic charge-transfer crystals. *Physical Review B*, **1986**, 34, 2131-2139	3.3	58
157	Accurate electron-molecular vibration coupling constants from powders optical spectra: TCNQ and TTF. *Solid State Communications*, **1984**, 52, 801-806	1.6	57
156	Intra- and intermolecular charge transfer in aggregates of tetrathiafulvalene-triphenylmethyl radical derivatives in solution. *Journal of the American Chemical Society*, **2013**, 135, 6958-67	16.4	56
155	Bistability in Fc-PTM crystals: the role of intermolecular electrostatic interactions. *Journal of the American Chemical Society*, **2008**, 130, 12064-72	16.4	56

154	Solvation Effects and Inhomogeneous Broadening in Optical Spectra of Phenol Blue. *Journal of Physical Chemistry A*, **2000**, 104, 11049-11054	2.8	55
153	First hyperpolarizability dispersion of the octupolar molecule crystal violet: multiple resonances and vibrational and solvation effects. *Journal of the American Chemical Society*, **2010**, 132, 16467-78	16.4	54
152	Dielectric response of modified Hubbard models with neutral-ionic and Peierls transitions. *Journal of Chemical Physics*, **2004**, 120, 6712-20	3.9	49
151	Symmetry crossover and excitation thresholds at the neutral-ionic transition of the modified Hubbard model. *Physical Review B*, **2001**, 63,	3.3	47
150	Giant infrared intensity of the Peierls mode at the neutral-ionic phase transition. *Physical Review Letters*, **2002**, 89, 027402	7.4	47
149	Charge fluctuations and electron–phonon coupling in organic charge-transfer salts with neutral–ionic and Peierls transitions. *Synthetic Metals*, **2004**, 141, 129-138	3.6	46
148	Electron–phonon coupling in conjugated polymers: Reference force field and transferable coupling constants for polyacetylene. *Journal of Chemical Physics*, **1993**, 98, 7459-7465	3.9	45
147	Two-photon absorption spectra of a near-infrared 2-azaazulene polymethine dye: solvation and ground-state symmetry breaking. *Physical Chemistry Chemical Physics*, **2013**, 15, 7666-78	3.6	44
146	Mixed regular stack charge–transfer crystals: Fundamental microscopic parameters from optical spectra. *Journal of Chemical Physics*, **1987**, 87, 1705-1711	3.9	44
145	Ab initio estimate of Hubbard model parameters:mA simple procedure appliedto BEDT-TTF salts. *Physical Review B*, **1997**, 55, 16088-16095	3.3	43
144	Multielectron transfer in clusters of polar-polarizable chromophores. *Journal of the American Chemical Society*, **2003**, 125, 5624-5	16.4	43
143	Aggregates of quadrupolar dyes: giant two-photon absorption from biexciton states. *Journal of Physical Chemistry B*, **2006**, 110, 25590-2	3.4	42
142	Bistability of Fc-PTM-Based Dyads: The Role of the Donor Strength. *Chemistry of Materials*, **2013**, 25, 808-814	9.6	41
141	Essential state models for solvatochromism in donor-acceptor molecules: the role of the bridge. *Journal of Physical Chemistry B*, **2009**, 113, 4718-25	3.4	41
140	Aggregates of quadrupolar dyes for two-photon absorption: the role of intermolecular interactions. *Physical Chemistry Chemical Physics*, **2016**, 18, 28198-28208	3.6	40
139	Induced self-assembly of a tetrathiafulvalene-based open-shell dyad through intramolecular electron transfer. *Angewandte Chemie - International Edition*, **2012**, 51, 11024-8	16.4	39
138	Fluorescence anisotropy spectra disclose the role of disorder in optical spectra of branched intramolecular-charge-transfer molecules. *Journal of Physical Chemistry B*, **2011**, 115, 7009-20	3.4	38
137	Vibronic contributions to resonant NLO responses: two-photon absorption in push–pull chromophores. *Chemical Physics Letters*, **2001**, 346, 470-478	2.5	38

136	Dimers of polar chromophores in solution: role of excitonic interactions in one- and two-photon absorption properties. *Physical Chemistry Chemical Physics*, **2011**, 13, 11099-109	3.6	37
135	Electron-Intramolecular Phonon Coupling in regular and Dimerized Mixed Stack Organic Semiconductors. *Molecular Crystals and Liquid Crystals*, **1985**, 120, 17-26		35
134	From Solution to Langmuir Blodgett Films: Spectroscopic Study of a Zwitterionic Dye. *Journal of Physical Chemistry B*, **2004**, 108, 10743-10750	3.4	34
133	Cooperative interactions in supramolecular aggregates: linear and nonlinear responses in calix[4]arenes. *ChemPhysChem*, **2006**, 7, 2168-74	3.2	33
132	Metastable domains and potential energy surfaces in organic charge-transfer salts with neutral-ionic phase transitions. *Physical Review B*, **2007**, 75,	3.3	32
131	On the ab initio evaluation of Hubbard parameters. II. The (BEDT-TTF)2Cu[N(CN)2]Br crystal. *Journal of Chemical Physics*, **1997**, 106, 8051-8058	3.9	30
130	Thermomagnetic Molecular System Based on TTF-PTM Radical: Switching the Spin and Charge Delocalization. *Journal of Physical Chemistry Letters*, **2013**, 4, 2721-2726	6.4	29
129	Vibronic model for spin crossover complexes. *Physical Review B*, **2011**, 84,	3.3	29
128	Polarization in organic molecular crystals and charge-transfer salts. *Journal of Luminescence*, **2004**, 110, 332-341	3.8	28
127	CS2 TCNQ3 Revisited: A Detailed Description of its Ground State Through a Reinterpretation of the Optical Spectra. *Molecular Crystals and Liquid Crystals*, **1986**, 134, 1-19		28
126	Molecular Vibration Analysis of Ionicity and Phase Transition in TMPD-TCNQ (1:1) Charge Transfer Salt. *Molecular Crystals and Liquid Crystals*, **1984**, 112, 325-343		27
125	Asymmetric squaraine dyes: spectroscopic and theoretical investigation. *Journal of Physical Chemistry B*, **2013**, 117, 8536-46	3.4	26
124	Enhancing the efficiency of two-photon absorption by metal coordination. *Physical Chemistry Chemical Physics*, **2009**, 11, 9450-7	3.6	26
123	Static nonlinear optical susceptibilities: Testing approximation schemes against exact results. *Journal of Chemical Physics*, **2002**, 116, 755-761	3.9	26
122	Spectroscopic characterization and modeling of quadrupolar charge-transfer dyes with bulky substituents. *Journal of Physical Chemistry B*, **2012**, 116, 4959-66	3.4	23
121	Direct evidence of overdamped Peierls-coupled modes in the temperature-induced phase transition in tetrathiafulvalene-chloranil. *Physical Review B*, **2008**, 78,	3.3	23
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119	Linear and non-linear optical properties of push pull chromophores: vibronic and solvation effects beyond perturbation theory. *Synthetic Metals*, **2001**, 124, 171-173	3.6	22

118	Supramolecular chirality: a caveat in assigning the handedness of chiral aggregates. *Chemical Communications*, **2020**, 56, 8281-8284	5.8	21
117	Essential state model for two-photon absorption spectra of polymethine dyes. *ChemPhysChem*, **2012**, 13, 2795-800	3.2	21
116	Dimers of quadrupolar chromophores in solution: electrostatic interactions and optical spectra. *Journal of Physical Chemistry B*, **2010**, 114, 882-93	3.4	21
115	Exact numerical diagonalization of one-dimensional interacting electrons non-adiabatically coupled to phonons. *Europhysics Letters*, **1996**, 34, 127-132	1.6	21
114	Electron-transfer in molecular functional materials. *Theoretical Chemistry Accounts*, **2007**, 117, 915-931	1.9	21
113	Pariser□Parr□Pople force field for □electrons: Raman and infrared shifts of trans-polyacetylene. *Journal of Chemical Physics*, **1994**, 100, 7144-7152	3.9	21
112	Interacting electrons in 1D: Applicability of Hubbard models. *Synthetic Metals*, **1988**, 27, A15-A20	3.6	21
111	Cooperativity from electrostatic interactions: understanding bistability in molecular crystals. *CrystEngComm*, **2009**, 11, 2040	3.3	20
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106	□electron force field in internal coordinates for trans- and cis-polyacetylene. *Chemical Physics*, **1994**, 184, 139-148	2.3	18
105	Electron correlations in one dimension: The Hubbard model. *Physical Review B*, **1989**, 39, 2830-2833	3.3	18
104	Hubbard models and their applicability in solid state and molecular physics. *Solid State Communications*, **1988**, 66, 273-275	1.6	18
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102	About the origin of the large Stokes shift in aminoalkyl substituted heptamethine cyanine dyes. *Physical Chemistry Chemical Physics*, **2019**, 22, 129-135	3.6	17
101	Tuning the nature of the fluorescent state: a substituted polycondensed dye as a case study. *Chemistry - A European Journal*, **2013**, 19, 924-35	4.8	16

100	Spectroscopic Investigation and Theoretical Modeling of Benzothiadiazole-Based Charge-Transfer Chromophores: From Solution to Nanoaggregates. *Journal of Physical Chemistry C*, **2017**, 121, 17466-17478	3.8	16
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98	Halogen-bridged mixed valence Pt complexes: Comparison with mixed and segregated stack charge-transfer crystals. *Synthetic Metals*, **1989**, 29, 181-188	3.6	16
97	Two-dimensional electronic-vibrational spectra: modeling correlated electronic and nuclear motion. *Physical Chemistry Chemical Physics*, **2015**, 17, 13074-81	3.6	15
96	Nanostructuring Lipophilic Dyes in Water Using Stable Vesicles, Quatsomes, as Scaffolds and Their Use as Probes for Bioimaging. *Small*, **2018**, 14, e1703851	11	15
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94	Beyond the F□ster formulation for resonance energy transfer: the role of dark states. *Physical Chemistry Chemical Physics*, **2011**, 13, 12734-44	3.6	15
93	On the ab initio evaluation of Hubbard parameters. I. The analytical approach in the absence of orbital relaxation. *Journal of Chemical Physics*, **1997**, 106, 8041-8050	3.9	14
92	Anharmonicity and NLO responses: an exact diagonalization study. *Chemical Physics Letters*, **2001**, 338, 208-216	2.5	14
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88	Modeling the Neutral-Ionic Transition with Correlated Electrons Coupled to Soft Lattices and Molecules. *Crystals*, **2017**, 7, 144	2.3	12
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75	Cooperative and non-linear phenomena at the neutral–ionic phase transition. *Synthetic Metals*, **2003**, 133-134, 619-621	3.6	10
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63	Ultrafast spectroscopy, superluminescence and theoretical modeling of a two-photon absorbing fluorene derivative. *Physical Chemistry Chemical Physics*, **2016**, 18, 12839-46	3.6	9
62	Understanding TADF: a joint experimental and theoretical study of DMAC-TRZ. *Physical Chemistry Chemical Physics*, **2021**, 23, 378-387	3.6	9
61	Electronic Nature of Nonlinear Optical Properties of a Symmetrical Two-Photon Absorbing Fluorene Derivative: Experimental Study and Theoretical Modeling. *Journal of Physical Chemistry C*, **2018**, 122, 5664-5672	3.8	8
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55	Polyacetylene oligomers: □electron fluctuations, vibrational intensities, and soliton confinement. *Physical Review B*, **1999**, 60, 8129-8137	3.3	7
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40	IR excitation spectra of low dimensional CT crystals: Multidimensional linear response theory approach. *Solid State Communications*, **1987**, 63, 1087-1092	1.6	5
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31	Electron-Phonon Vs. Electron-Electron Interactions in Low Dimensional Solids. *Molecular Crystals and Liquid Crystals*, **1993**, 234, 145-154		3
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28	Phonon quantum fluctuations at the neutral-ionic transition Application of a new exact numerical technique for finite clusters. *Synthetic Metals*, **1991**, 43, 3619-3622	3.6	3
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20	Electron-phonon coupling in mixed-valence compounds: mode mixing and coupling constants. *The Journal of Physical Chemistry*, **1989**, 93, 8385-8386		2
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16	Static polarizability of molecular materials: Environmental and vibrational contributions. *Journal of Computational Methods in Sciences and Engineering*, **2004**, 4, 703-720	0.3	1
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11	Increasing resonance energy transfer upon dilution: a counterintuitive observation in CTAB micelles. *Journal of Materials Chemistry C*, **2021**, 9, 10952-10964	7.1	0

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10	Vibrational spectra of pristine, photoexcited and doped polyacetylene: towards a microscopic model. *Synthetic Metals*, **1997**, 85, 1079-1080	3.6
9	Charge transfer processes and environmental degrees of freedom: cooperativity and non-linearity. *Macromolecular Symposia*, **2004**, 212, 123-130	0.8
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6	Comment on: The instabilities of mixed stack organic charge transfer crystals. *Journal of Chemical Physics*, **1988**, 89, 616-617	3.9
5	Charge instabilities in molecular materials: cooperative behavior from electrostatic interactions **2005**, 129-141	
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3	Beyond the Hubbard Model: Screened Interactions in 1D. *NATO ASI Series Series B: Physics*, **1990**, 441-446	
2	REGULAR-DIMERIZED STACK vs NEUTRAL-IONIC INSTABILITY IN MIXED STACK CT CRYSTALS **1986**, 559-561	
1	Mean-Field Effects on the Phosphorescence of Dinuclear Re(I) Complex Polymorphs.. *Crystal Growth and Design*, **2022**, 22, 772-778	3.5