Guido Raos

List of Publications by Year
in descending order

103 papers	3,377 citations	159585 30 h-index	161849 54 g-index
105 all docs	105 docs citations	105 times ranked	3923 citing authors

#	Article	IF	Citations
1	Theories and simulations of polymer-based nanocomposites: From chain statistics to reinforcement. Progress in Polymer Science, 2008, 33, 683-731.	24.7	256
2	Interaction of Water with the Model Ionic Liquid [bmim][BF₄]: Molecular Dynamics Simulations and Comparison with NMR Data. Journal of Physical Chemistry B, 2008, 112, 7826-7836.	2.6	231
3	Halogen Bonding in Fluoroalkylhalides:Â A Quantum Chemical Study of Increasing Fluorine Substitution. Journal of Physical Chemistry A, 2000, 104, 1617-1620.	2.5	198
4	The Local Structure of Ionic Liquids: Cationâ€“Cation NOE Interactions and Internuclear Distances in Neat [BMIM][BF4] and [BDMIM][BF4]. Angewandte Chemie - International Edition, 2006, 45, 1123-1126.	13.8	142
5	Computational reinvestigation of the bithiophene torsion potential. Chemical Physics Letters, 2003, 379, 364-372.	2.6	121
6	Computational Experiments on Filled Rubber Viscoelasticity:Â What Is the Role of Particleâ^'Particle Interactions?. Macromolecules, 2006, 39, 6744-6751.	4.8	104
7	Structural Organization and Transport Properties of Novel Pyrrolidinium-Based Ionic Liquids with Perfluoroalkyl Sulfonylimide Anions. Journal of Physical Chemistry B, 2009, 113, 10750-10759.	2.6	102
8	Side-Chain Role in Chemically Sensing Conducting Polymer Field-Effect Transistors. Journal of Physical Chemistry B, 2003, 107, 7589-7594.	2.6	101
9	Molecular Modeling of Crystalline Alkylthiophene Oligomers and Polymers. Journal of Physical Chemistry B, 2010, 114, 1591-1602.	2.6	87
10	Methodological assessment of kinetic Monte Carlo simulations of organic photovoltaic devices: The treatment of electrostatic interactions. Journal of Chemical Physics, 2010, 132, 094705.	3.0	74
11	Organicâ^'Organic Epitaxy of Incommensurate Systems:Â Quaterthiophene on Potassium Hydrogen Phthalate Single Crystals. Journal of the American Chemical Society, 2006, 128, 13378-13387.	13.7	71
12	Molecular Modeling of Crystalline Oligothiophenes:Â Testing and Development of Improved Force Fields. Journal of Physical Chemistry B, 2004, 108, 18053-18064.	2.6	69
13	Blending ionic liquids: how physico-chemical properties change. Physical Chemistry Chemical Physics, 2010, 12, 1784.	2.8	69
14	Free Energies of Molecular Crystal Surfaces by Computer Simulation:Â Application to Tetrathiophene. Journal of the American Chemical Society, 2006, 128, 1408-1409.	13.7	63
15	Pyrrolidinium-Based Ionic Liquids Doped with Lithium Salts: How Does Li⁺ Coordination Affect Its Diffusivity?. Journal of Physical Chemistry B, 2014, 118, 13679-13688.	2.6	63
16	Polymer Adhesion: Seeking New Solutions for an Old Problem. Macromolecules, 2021, 54, 10617-10644.	4.8	59
17	Chain collapse and phase separation in poorâ€solvent polymer solutions: A unified molecular description. Journal of Chemical Physics, 1996, 104, 1626-1645.	3.0	54
18	Ordered Stacking of Regioregular Head-to-Tail Polyalkylthiophenes: Insights from the Crystal Structure of Form Iâ€² Poly(3-n-butylthiophene). Chemistry of Materials, 2009, 21, 78-87.	6.7	50

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19	Nonequilibrium simulations of filled polymer networks: Searching for the origins of reinforcement and nonlinearity. Journal of Chemical Physics, 2011, 134, 054902.	3.0	50
20	Pyrazolium- versus Imidazolium-Based Ionic Liquids: Structure, Dynamics and Physicochemical Properties. Journal of Physical Chemistry B, 2013, 117, 668-676.	2.6	49
21	Modeling of Molecular Packing and Conformation in Oligofluorenes. Journal of Physical Chemistry B, 2006, 110, 5253-5261.	2.6	48
22	Solvent-free phenyl-C61-butyric acid methyl ester (PCBM) from clathrates: insights for organic photovoltaics from crystal structures and molecular dynamics. Chemical Communications, 2013, 49, 4525.	4.1	47
23	Interplay of Conformational States and Nonbonded Interactions in Substituted Bithiophenes. Journal of Physical Chemistry A, 2004, 108, 691-698.	2.5	44
24	Form II Poly(3-butylthiophene): Crystal Structure and Preferred Orientation in Spherulitic Thin Films. Macromolecules, 2010, 43, 6772-6781.	4.8	43
25	Electron transport in crystalline PCBM-like fullerene derivatives: a comparative computational study. Journal of Materials Chemistry C, 2014, 2, 7313-7325.	5.5	41
26	Macromolecular clusters in poor-solvent polymer solutions. Journal of Chemical Physics, 1997, 107, 6479-6490.	3.0	39
27	Pair populations and effective valencies from ab initio SCF and spin-coupled wave functions. International Journal of Quantum Chemistry, 1996, 57, 501-518.	2.0	36
28	Incommensurate Epitaxy of Tetrathiophene on Potassium Hydrogen Phthalate:â€‰ Insights from Molecular Simulation. Crystal Growth and Design, 2006, 6, 1826-1832.	3.0	34
29	Application of the Christensen-Lo Model to the Reinforcement of Elastomers by Fractal Fillers. Macromolecular Theory and Simulations, 2003, 12, 17-23.	1.4	33
30	Strategies for two-dimensional growth of organic molecular films. Chemical Physics, 2006, 325, 193-206.	1.9	33
31	Intramolecular CH/Ï€ interactions in alkylaromatics: Monomer conformations for poly(3â€alkylthiophene) atomistic models. International Journal of Quantum Chemistry, 2013, 113, 2154-2162.	2.0	31
32	On the role of different spin bases within spin-coupled theory. Molecular Physics, 1993, 79, 197-216.	1.7	29
33	Molecular dynamics simulations of the solvent- and thermal history-dependent structure of the PCBM fullerene derivative. Journal of Materials Chemistry, 2012, 22, 5434.	6.7	29
34	The Lowest Singlet and Triplet States of oâ€Benzyne: Spinâ€Coupled Interpretation of the Electronic Structure at CAS SCF Equilibrium Geometries. Israel Journal of Chemistry, 1993, 33, 253-264.	2.3	27
35	A Solid State Density Functional Study of Crystalline Thiophene-Based Oligomers and Polymers. Journal of Physical Chemistry B, 2012, 116, 14504-14509.	2.6	27
36	Coarseâ€Grained Simulations of Model Polymer Nanofibres. Macromolecular Theory and Simulations, 2011, 20, 305-319.	1.4	26

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37	A Cluster of Chains Can Be Smaller Than a Single Chain:Â New Interpretation of Kinetics of Collapse Experiments. Macromolecules, 1996, 29, 8565-8567.	4.8	24
38	From Nanoscale to Microscale: Crossover in the Diffusion Dynamics within Two Pyrrolidinium-Based Ionic Liquids. Journal of Physical Chemistry Letters, 2017, 8, 5196-5202.	4.6	23
39	Molecular dynamics simulation of rupture in glassy polymer bridges within filler aggregates. Physical Review E, 2012, 86, 041801.	2.1	22
40	Improving the efficiency of P3HT:perylene diimide solar cells via bay-substitution with fused aromatic rings. RSC Advances, 2013, 3, 9185.	3.6	22
41	An Effective Two-Orbital Quantum Chemical Model for Organic Photovoltaic Materials. Journal of Chemical Theory and Computation, 2014, 10, 364-372.	5.3	21
42	Tetrathiophene on Graphite: Molecular Dynamics Simulations. Macromolecular Theory and Simulations, 2004, 13, 497-505.	1.4	20
43	Numerical simulation of photocurrent generation in bilayer organic solar cells: Comparison of master equation and kinetic Monte Carlo approaches. Journal of Chemical Physics, 2013, 139, 024706.	3.0	20
44	Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. I. Theory and first applications. Chemical Physics, 1994, 186, 233-250.	1.9	19
45	Structure of an Associating Polymer Melt in a Narrow Slit by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2005, 109, 18117-18126.	2.6	19
46	Conformational Analysis of 2,2â€˜-Bithiophene:Â A1H Liquid Crystal NMR Study Using the13C Satellite Spectra. Journal of Physical Chemistry A, 2005, 109, 9953-9963.	2.5	19
47	Role of Desorption in the Growth Process of Molecular Organic Thin Films. Journal of Physical Chemistry B, 2005, 109, 7859-7864.	2.6	19
48	Atomistic Simulation of Phase Transitions and Charge Mobility for the Organic Semiconductor Ph-BTBT-C10. Chemistry of Materials, 2019, 31, 7092-7103.	6.7	19
49	Viscoelasticity of Short Polymer Liquids from Atomistic Simulations. Journal of the Electrochemical Society, 2019, 166, B3246-B3256.	2.9	19
50	Spin-Coupled Study of the Electronic Structure of Polyenyl Radicals C3H5-C9H11. Journal of the American Chemical Society, 1994, 116, 2075-2084.	13.7	18
51	Polymer association in poor solvents: from monomolecular micelles to clusters of chains and phase separation. Macromolecular Theory and Simulations, 1999, 8, 65-84.	1.4	18
52	Mesoscopic bead-and-spring model of hard spherical particles in a rubber matrix. I. Hydrodynamic reinforcement. Journal of Chemical Physics, 2000, 113, 7554-7563.	3.0	18
53	The collapse of chains with different architectures. Journal of Chemical Physics, 1994, 100, 7804-7813.	3.0	17
54	Structure of Model Telechelic Polymer Melts by Computer Simulation. Journal of Macromolecular Science - Physics, 2005, 44, 855-871.	1.0	17

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55	Impact of Interaction Strength and Surface Heterogeneity on the Dynamics of Adsorbed Polymers. ACS Macro Letters, 2014, 3, 721-726.	4.8	17
56	Spin-Coupled Valence Bond Study of the Reaction between Benzene and a Methyl Cation. Journal of Physical Chemistry A, 1997, 101, 2886-2892.	2.5	16
57	Effects of chemically heterogeneous nanoparticles on polymer dynamics: insights from molecular dynamics simulations. Soft Matter, 2018, 14, 1219-1226.	2.7	16
58	Glassy dynamics of a polymer monolayer on a heterogeneous disordered substrate. Soft Matter, 2015, 11, 8083-8091.	2.7	15
59	Influence of wall heterogeneity on nanoscopically confined polymers. Physical Chemistry Chemical Physics, 2019, 21, 772-779.	2.8	15
60	Antiferromagnetic Spin Couplings in Cyclobutadiene Chains. Journal of Physical Chemistry B, 1997, 101, 6688-6691.	2.6	14
61	Hydrophobic aggregation and collective absorption of dioxin into lipid membranes: insights from atomistic simulations. Physical Chemistry Chemical Physics, 2015, 17, 2344-2348.	2.8	14
62	Molecular dynamics simulation of metallic impurity diffusion in liquid lead-bismuth eutectic (LBE). Journal of Nuclear Materials, 2018, 501, 253-260.	2.7	14
63	Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. II. Further applications. Chemical Physics, 1994, 186, 251-273.	1.9	13
64	Chain Interactions in Poor-Solvent Polymer Solutions:â€‰ Equilibrium and Nonequilibrium Aspects. Macromolecules, 1996, 29, 6663-6670.	4.8	13
65	Degrees of Chirality in Helical Structures. Macromolecular Theory and Simulations, 2002, 11, 739-750.	1.4	13
66	Functionalized Oligothiophenes for Optoelectronic Applications:â€‰ 3â€˜,4â€˜,3â€˜â€‰â€˜â€˜,4â€˜â€‰â€˜â€˜-Tetra [(methoxycarbonyl)methyl]-2,2â€˜:5â€˜,2â€˜â€‰â€˜:5â€˜â€‰â€˜,2â€˜â€‰â€˜â€˜:5â€˜â€‰â€˜â€˜,2â€˜â€‰â€˜â€˜â€‰â€˜â€˜-quinquithi Materials, 2005, 17, 242-249.	6.7	13
67	Organic Peracids: A Structural Puzzle for ¹⁷O NMR and Ab Initio Chemical Shift Calculations. Journal of Physical Chemistry A, 2012, 116, 1814-1819.	2.5	13
68	Coarse-grained kinetic modelling of bilayer heterojunction organic solar cells. Organic Electronics, 2012, 13, 750-761.	2.6	13
69	Evidence of superdiffusive nanoscale motion in anionic polymeric hydrogels: Analysis of PGSE- NMR data and comparison with drug release properties. Journal of Controlled Release, 2019, 305, 110-119.	9.9	13
70	A Coarse-Grained Force Field for Silicaâ€“Polybutadiene Interfaces and Nanocomposites. Polymers, 2020, 12, 1484.	4.5	12
71	Aromatic electrophilic substitution. A modern valence bond study. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4011.	1.7	11
72	Origin of Charge Separation at Organic Photovoltaic Heterojunctions: A Mesoscale Quantum Mechanical View. Journal of Physical Chemistry C, 2017, 121, 16693-16701.	3.1	10

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73	All-Atom Model of Atactic 2-Vinyl Pyridine Polymer: Structural Properties Investigation by Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2019, 166, B3309-B3315.	2.9	10
74	Rigid filler particles in a rubber matrix: effective force constants by multipolar expansion. Computational and Theoretical Polymer Science, 2000, 10, 149-157.	1.1	9
75	Materials for organic photovoltaics: insights from detailed structural models and molecular simulations. EPJ Web of Conferences, 2012, 33, 02002.	0.3	9
76	Pulling Polymers on Energetically Disordered Surfaces: Molecular Dynamics Tests of Linear and Nonâ€linear Response. Macromolecular Theory and Simulations, 2013, 22, 225-237.	1.4	9
77	Fracture in Silica/Butadiene Rubber: A Molecular Dynamics View of Designâ€“Property Relationships. ACS Polymers Au, 0, , .	4.1	9
78	Sliding friction between polymer surfaces: A molecular interpretation. Journal of Chemical Physics, 2006, 124, 144713.	3.0	8
79	Equilibrium Dynamics of an Associating Polymer Melt in Narrow Slits by Computer Simulation. Journal of Physical Chemistry B, 2007, 111, 4141-4149.	2.6	8
80	Computational 17O-NMRspectroscopy of organic acids and peracids: comparison of solvation models. Physical Chemistry Chemical Physics, 2013, 15, 1130-1140.	2.8	8
81	The effect of donor content on the efficiency of P3HT:PCBM bilayers: optical and photocurrent spectral data analyses. Physical Chemistry Chemical Physics, 2015, 17, 2447-2456.	2.8	8
82	Molecular Dynamics Simulation on Physical Properties of Liquid Lead, Bismuth and Lead-bismuth Eutectic (LBE). Procedia Engineering, 2016, 157, 214-221.	1.2	8
83	Atomistic modelling of entropy driven phase transitions between different crystal modifications in polymers: the case of poly(3-alkylthiophenes). Physical Chemistry Chemical Physics, 2018, 20, 28984-28989.	2.8	8
84	Magnetic Resonance Imaging and Molecular Dynamics Characterization of Ionic Liquid in Poly(ethylene oxide)-Based Polymer Electrolytes. ACS Applied Materials & Interfaces, 2020, 12, 23800-23811.	8.0	8
85	Catalytic chemistry of furan and thiophene. Ab initio calculations, using the spin-coupled valence bond method, of the interaction of furan and thiophene with a positively charged centre. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 749.	1.7	7
86	Stereochemically pure Î±-trifluoromethyl-malic hydroxamates: synthesis and evaluation as inhibitors of matrix metalloproteinases. Tetrahedron, 2006, 62, 10171-10181.	1.9	7
87	17O NMR. Annual Reports on NMR Spectroscopy, 2015, 85, 143-193.	1.5	7
88	From dioxin to dioxin congeners: understanding the differences in hydrophobic aggregation in water and absorption into lipid membranes by means of atomistic simulations. Physical Chemistry Chemical Physics, 2016, 18, 17731-17739.	2.8	7
89	Surface Reconstructions in Organic Crystals: Simulations of the Effect of Temperature and Defectivity on Bulk and (001) Surfaces of 2,2â€²:6â€²,2â€³-Ternaphthalene. Crystal Growth and Design, 2016, 16, 412-422.	3.0	7
90	Towards realistic simulations of polymer networks: tuning vulcanisation and mechanical properties. Physical Chemistry Chemical Physics, 2021, 23, 3496-3510.	2.8	7

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91	Rigid particles in an elastic polymer network: An electrical-analog approach. Journal of Chemical Physics, 1998, 109, 3285-3292.	3.0	6
92	Rotational barriers of amides and polyisocyanates: A spin-coupled study. International Journal of Quantum Chemistry, 1999, 74, 249-258.	2.0	6
93	Confined polymer networks: The harmonic approach. Journal of Chemical Physics, 2002, 116, 3109-3118.	3.0	6
94	Polymer-mediated adhesion: A statistical approach. Journal of Chemical Physics, 2003, 119, 9295-9307.	3.0	6
95	Association and Diffusion of Li⁺ in Carboxymethylcellulose Solutions for Environmentally Friendly Liâ€ion Batteries. ChemSusChem, 2016, 9, 1804-1813.	6.8	6
96	Tunable interaction potentials and morphology of polymerâ€“nanoparticle blends. Journal of Chemical Physics, 2020, 152, 174902.	3.0	5
97	Quo Vadis, Macromolecular Science? Reflections by the IUPAC Polymer Division on the Occasion of the Staudinger Centenary. Israel Journal of Chemistry, 2020, 60, 9-19.	2.3	5
98	Identification of viable TCDD access pathways to human AhR PAS-B ligand binding domain. Journal of Molecular Graphics and Modelling, 2021, 105, 107886.	2.4	5
99	Polymer-Mediated Adhesion: Nanoscale Surface Morphology and Failure Mechanisms. Macromolecules, 2021, 54, 195-202.	4.8	4
100	Substituent effects on the second-order hyperpolarisability of cyanine cations. Computational and Theoretical Chemistry, 2002, 589-590, 439-445.	1.5	3
101	Rubber elasticity: A contactâ€probability model with harmonic entanglement constraints. Journal of Chemical Physics, 1996, 105, 8352-8361.	3.0	2
102	Polymer Chains and Networks in Narrow Slits. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2005, , 249-268.	0.1	0
103	Viscoelasticity of Short Polymer Melts from Atomistic Simulations. ECS Meeting Abstracts, 2018, , .	0.0	0