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	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
2	Towards realistic simulations of polymer networks: tuning vulcanisation and mechanical properties. Physical Chemistry Chemical Physics, 2021, 23, 3496-3510.	2.8	7
3	Polymer-Mediated Adhesion: Nanoscale Surface Morphology and Failure Mechanisms. Macromolecules, 2021, 54, 195-202.	4.8	4
4	Polymer Adhesion: Seeking New Solutions for an Old Problem. Macromolecules, 2021, 54, 10617-10644.	4.8	59
5	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
6	Tunable interaction potentials and morphology of polymerâ€“nanoparticle blends. Journal of Chemical Physics, 2020, 152, 174902.	3.0	5
7	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
8	A Coarse-Grained Force Field for Silicaâ€“Polybutadiene Interfaces and Nanocomposites. Polymers, 2020, 12, 1484.	4.5	12
9	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
10	Influence of wall heterogeneity on nanoscopically confined polymers. Physical Chemistry Chemical Physics, 2019, 21, 772-779.	2.8	15
11	Viscoelasticity of Short Polymer Liquids from Atomistic Simulations. Journal of the Electrochemical Society, 2019, 166, B3246-B3256.	2.9	19
12	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
13	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
14	Molecular dynamics simulation of metallic impurity diffusion in liquid lead-bismuth eutectic (LBE). Journal of Nuclear Materials, 2018, 501, 253-260.	2.7	14
15	Effects of chemically heterogeneous nanoparticles on polymer dynamics: insights from molecular dynamics simulations. Soft Matter, 2018, 14, 1219-1226.	2.7	16
16	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
17	Viscoelasticity of Short Polymer Melts from Atomistic Simulations. ECS Meeting Abstracts, 2018, , .	0.0	0
18	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

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19	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
20	Association and Diffusion of Li⁺ in Carboxymethylcellulose Solutions for Environmentally Friendly Liâ€ion Batteries. ChemSusChem, 2016, 9, 1804-1813.	6.8	6
21	Molecular Dynamics Simulation on Physical Properties of Liquid Lead, Bismuth and Lead-bismuth Eutectic (LBE). Procedia Engineering, 2016, 157, 214-221.	1.2	8
22	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
23	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
24	17O NMR. Annual Reports on NMR Spectroscopy, 2015, 85, 143-193.	1.5	7
25	Glassy dynamics of a polymer monolayer on a heterogeneous disordered substrate. Soft Matter, 2015, 11, 8083-8091.	2.7	15
26	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
27	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
28	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
29	An Effective Two-Orbital Quantum Chemical Model for Organic Photovoltaic Materials. Journal of Chemical Theory and Computation, 2014, 10, 364-372.	5.3	21
30	Electron transport in crystalline PCBM-like fullerene derivatives: a comparative computational study. Journal of Materials Chemistry C, 2014, 2, 7313-7325.	5.5	41
31	Impact of Interaction Strength and Surface Heterogeneity on the Dynamics of Adsorbed Polymers. ACS Macro Letters, 2014, 3, 721-726.	4.8	17
32	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
33	Computational 17O-NMRspectroscopy of organic acids and peracids: comparison of solvation models. Physical Chemistry Chemical Physics, 2013, 15, 1130-1140.	2.8	8
34	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
35	Pyrazolium- versus Imidazolium-Based Ionic Liquids: Structure, Dynamics and Physicochemical Properties. Journal of Physical Chemistry B, 2013, 117, 668-676.	2.6	49
36	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

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37	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
38	Improving the efficiency of P3HT:perylene diimide solar cells via bay-substitution with fused aromatic rings. RSC Advances, 2013, 3, 9185.	3.6	22
39	Materials for organic photovoltaics: insights from detailed structural models and molecular simulations. EPJ Web of Conferences, 2012, 33, 02002.	0.3	9
40	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
41	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
42	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
43	Molecular dynamics simulation of rupture in glassy polymer bridges within filler aggregates. Physical Review E, 2012, 86, 041801.	2.1	22
44	Coarse-grained kinetic modelling of bilayer heterojunction organic solar cells. Organic Electronics, 2012, 13, 750-761.	2.6	13
45	Nonequilibrium simulations of filled polymer networks: Searching for the origins of reinforcement and nonlinearity. Journal of Chemical Physics, 2011, 134, 054902.	3.0	50
46	Coarseâ€Grained Simulations of Model Polymer Nanofibres. Macromolecular Theory and Simulations, 2011, 20, 305-319.	1.4	26
47	Molecular Modeling of Crystalline Alkylthiophene Oligomers and Polymers. Journal of Physical Chemistry B, 2010, 114, 1591-1602.	2.6	87
48	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
49	Blending ionic liquids: how physico-chemical properties change. Physical Chemistry Chemical Physics, 2010, 12, 1784.	2.8	69
50	Form II Poly(3-butylthiophene): Crystal Structure and Preferred Orientation in Spherulitic Thin Films. Macromolecules, 2010, 43, 6772-6781.	4.8	43
51	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
52	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
53	Theories and simulations of polymer-based nanocomposites: From chain statistics to reinforcement. Progress in Polymer Science, 2008, 33, 683-731.	24.7	256
54	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

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55	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
56	Incommensurate Epitaxy of Tetrathiophene on Potassium Hydrogen Phthalate:â€‰ Insights from Molecular Simulation. Crystal Growth and Design, 2006, 6, 1826-1832.	3.0	34
57	Computational Experiments on Filled Rubber Viscoelasticity:Â What Is the Role of Particleâ^'Particle Interactions?. Macromolecules, 2006, 39, 6744-6751.	4.8	104
58	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
59	Modeling of Molecular Packing and Conformation in Oligofluorenes. Journal of Physical Chemistry B, 2006, 110, 5253-5261.	2.6	48
60	Strategies for two-dimensional growth of organic molecular films. Chemical Physics, 2006, 325, 193-206.	1.9	33
61	Stereochemically pure Î±-trifluoromethyl-malic hydroxamates: synthesis and evaluation as inhibitors of matrix metalloproteinases. Tetrahedron, 2006, 62, 10171-10181.	1.9	7
62	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
63	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
64	Sliding friction between polymer surfaces: A molecular interpretation. Journal of Chemical Physics, 2006, 124, 144713.	3.0	8
65	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
66	Structure of Model Telechelic Polymer Melts by Computer Simulation. Journal of Macromolecular Science - Physics, 2005, 44, 855-871.	1.0	17
67	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	18
68	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
69	Role of Desorption in the Growth Process of Molecular Organic Thin Films. Journal of Physical Chemistry B, 2005, 109, 7859-7864.	2.6	19
70	Polymer Chains and Networks in Narrow Slits. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2005, , 249-268.	0.1	0
71	Tetrathiophene on Graphite: Molecular Dynamics Simulations. Macromolecular Theory and Simulations, 2004, 13, 497-505.	1.4	20
72	Interplay of Conformational States and Nonbonded Interactions in Substituted Bithiophenes. Journal of Physical Chemistry A, 2004, 108, 691-698.	2.5	44

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73	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
74	Computational reinvestigation of the bithiophene torsion potential. Chemical Physics Letters, 2003, 379, 364-372.	2.6	121
75	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
76	Side-Chain Role in Chemically Sensing Conducting Polymer Field-Effect Transistors. Journal of Physical Chemistry B, 2003, 107, 7589-7594.	2.6	101
77	Polymer-mediated adhesion: A statistical approach. Journal of Chemical Physics, 2003, 119, 9295-9307.	3.0	6
78	Confined polymer networks: The harmonic approach. Journal of Chemical Physics, 2002, 116, 3109-3118.	3.0	6
79	Degrees of Chirality in Helical Structures. Macromolecular Theory and Simulations, 2002, 11, 739-750.	1.4	13
80	Substituent effects on the second-order hyperpolarisability of cyanine cations. Computational and Theoretical Chemistry, 2002, 589-590, 439-445.	1.5	3
81	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
82	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
83	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
84	Rotational barriers of amides and polyisocyanates: A spin-coupled study. International Journal of Quantum Chemistry, 1999, 74, 249-258.	2.0	6
85	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
86	Rigid particles in an elastic polymer network: An electrical-analog approach. Journal of Chemical Physics, 1998, 109, 3285-3292.	3.0	6
87	Antiferromagnetic Spin Couplings in Cyclobutadiene Chains. Journal of Physical Chemistry B, 1997, 101, 6688-6691.	2.6	14
88	Macromolecular clusters in poor-solvent polymer solutions. Journal of Chemical Physics, 1997, 107, 6479-6490.	3.0	39
89	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
90	Chain Interactions in Poor-Solvent Polymer Solutions:â€‰ Equilibrium and Nonequilibrium Aspects. Macromolecules, 1996, 29, 6663-6670.	4.8	13

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91	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
92	Rubber elasticity: A contactâ€probability model with harmonic entanglement constraints. Journal of Chemical Physics, 1996, 105, 8352-8361.	3.0	2
93	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
94	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
95	Aromatic electrophilic substitution. A modern valence bond study. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4011.	1.7	11
96	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
97	The collapse of chains with different architectures. Journal of Chemical Physics, 1994, 100, 7804-7813.	3.0	17
98	Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. II. Further applications. Chemical Physics, 1994, 186, 251-273.	1.9	13
99	Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. I. Theory and first applications. Chemical Physics, 1994, 186, 233-250.	1.9	19
100	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
101	On the role of different spin bases within spin-coupled theory. Molecular Physics, 1993, 79, 197-216.	1.7	29
102	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
103	Fracture in Silica/Butadiene Rubber: A Molecular Dynamics View of Designâ€“Property Relationships. ACS Polymers Au, 0, , .	4.1	9