

Guido Raos

List of Publications by Year in descending order

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103
papers

3,377
citations

159358

30
h-index

161609

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. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107886.	1.3	5
2	Towards realistic simulations of polymer networks: tuning vulcanisation and mechanical properties. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3496-3510.	1.3	7
3	Polymer-Mediated Adhesion: Nanoscale Surface Morphology and Failure Mechanisms. <i>Macromolecules</i> , 2021, 54, 195-202.	2.2	4
4	Polymer Adhesion: Seeking New Solutions for an Old Problem. <i>Macromolecules</i> , 2021, 54, 10617-10644.	2.2	59
5	Magnetic Resonance Imaging and Molecular Dynamics Characterization of Ionic Liquid in Poly(ethylene oxide)-Based Polymer Electrolytes. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 23800-23811.	4.0	8
6	Tunable interaction potentials and morphology of polymer-nanoparticle blends. <i>Journal of Chemical Physics</i> , 2020, 152, 174902.	1.2	5
7	Quo Vadis, Macromolecular Science? Reflections by the IUPAC Polymer Division on the Occasion of the Staudinger Centenary. <i>Israel Journal of Chemistry</i> , 2020, 60, 9-19.	1.0	5
8	A Coarse-Grained Force Field for Silica-Polybutadiene Interfaces and Nanocomposites. <i>Polymers</i> , 2020, 12, 1484.	2.0	12
9	Atomistic Simulation of Phase Transitions and Charge Mobility for the Organic Semiconductor Ph-BTBT-C10. <i>Chemistry of Materials</i> , 2019, 31, 7092-7103.	3.2	19
10	Influence of wall heterogeneity on nanoscopically confined polymers. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 772-779.	1.3	15
11	Viscoelasticity of Short Polymer Liquids from Atomistic Simulations. <i>Journal of the Electrochemical Society</i> , 2019, 166, B3246-B3256.	1.3	19
12	All-Atom Model of Atactic 2-Vinyl Pyridine Polymer: Structural Properties Investigation by Molecular Dynamics Simulations. <i>Journal of the Electrochemical Society</i> , 2019, 166, B3309-B3315.	1.3	10
13	Evidence of superdiffusive nanoscale motion in anionic polymeric hydrogels: Analysis of PGSE- NMR data and comparison with drug release properties. <i>Journal of Controlled Release</i> , 2019, 305, 110-119.	4.8	13
14	Molecular dynamics simulation of metallic impurity diffusion in liquid lead-bismuth eutectic (LBE). <i>Journal of Nuclear Materials</i> , 2018, 501, 253-260.	1.3	14
15	Effects of chemically heterogeneous nanoparticles on polymer dynamics: insights from molecular dynamics simulations. <i>Soft Matter</i> , 2018, 14, 1219-1226.	1.2	16
16	Atomistic modelling of entropy driven phase transitions between different crystal modifications in polymers: the case of poly(3-alkylthiophenes). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28984-28989.	1.3	8
17	Viscoelasticity of Short Polymer Melts from Atomistic Simulations. <i>ECS Meeting Abstracts</i> , 2018, , .	0.0	0
18	From Nanoscale to Microscale: Crossover in the Diffusion Dynamics within Two Pyrrolidinium-Based Ionic Liquids. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5196-5202.	2.1	23

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19	Origin of Charge Separation at Organic Photovoltaic Heterojunctions: A Mesoscale Quantum Mechanical View. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16693-16701.	1.5	10
20	Association and Diffusion of Li ⁺ in Carboxymethylcellulose Solutions for Environmentally Friendly Li-ion Batteries. <i>ChemSusChem</i> , 2016, 9, 1804-1813.	3.6	6
21	Molecular Dynamics Simulation on Physical Properties of Liquid Lead, Bismuth and Lead-bismuth Eutectic (LBE). <i>Procedia Engineering</i> , 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. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17731-17739.	1.3	7
23	Surface Reconstructions in Organic Crystals: Simulations of the Effect of Temperature and Defectivity on Bulk and (001) Surfaces of 2,2,6,6-Tetraphenyl-2,2,6,6-Tetranaphthalene. <i>Crystal Growth and Design</i> , 2016, 16, 412-422.	1.4	7
24	17O NMR. <i>Annual Reports on NMR Spectroscopy</i> , 2015, 85, 143-193.	0.7	7
25	Glassy dynamics of a polymer monolayer on a heterogeneous disordered substrate. <i>Soft Matter</i> , 2015, 11, 8083-8091.	1.2	15
26	Hydrophobic aggregation and collective absorption of dioxin into lipid membranes: insights from atomistic simulations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2344-2348.	1.3	14
27	The effect of donor content on the efficiency of P3HT:PCBM bilayers: optical and photocurrent spectral data analyses. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2447-2456.	1.3	8
28	Pyrrrolidinium-Based Ionic Liquids Doped with Lithium Salts: How Does Li ⁺ Coordination Affect Its Diffusivity?. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13679-13688.	1.2	63
29	An Effective Two-Orbital Quantum Chemical Model for Organic Photovoltaic Materials. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 364-372.	2.3	21
30	Electron transport in crystalline PCBM-like fullerene derivatives: a comparative computational study. <i>Journal of Materials Chemistry C</i> , 2014, 2, 7313-7325.	2.7	41
31	Impact of Interaction Strength and Surface Heterogeneity on the Dynamics of Adsorbed Polymers. <i>ACS Macro Letters</i> , 2014, 3, 721-726.	2.3	17
32	Numerical simulation of photocurrent generation in bilayer organic solar cells: Comparison of master equation and kinetic Monte Carlo approaches. <i>Journal of Chemical Physics</i> , 2013, 139, 024706.	1.2	20
33	Computational 17O-NMR spectroscopy of organic acids and peracids: comparison of solvation models. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1130-1140.	1.3	8
34	Intramolecular CH/π interactions in alkylaromatics: Monomer conformations for poly(3-alkylthiophene) atomistic models. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2154-2162.	1.0	31
35	Pyrazolium- versus Imidazolium-Based Ionic Liquids: Structure, Dynamics and Physicochemical Properties. <i>Journal of Physical Chemistry B</i> , 2013, 117, 668-676.	1.2	49
36	Solvent-free phenyl-C61-butyric acid methyl ester (PCBM) from clathrates: insights for organic photovoltaics from crystal structures and molecular dynamics. <i>Chemical Communications</i> , 2013, 49, 4525.	2.2	47

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37	Pulling Polymers on Energetically Disordered Surfaces: Molecular Dynamics Tests of Linear and Nonlinear Response. <i>Macromolecular Theory and Simulations</i> , 2013, 22, 225-237.	0.6	9
38	Improving the efficiency of P3HT:perylene diimide solar cells via bay-substitution with fused aromatic rings. <i>RSC Advances</i> , 2013, 3, 9185.	1.7	22
39	Materials for organic photovoltaics: insights from detailed structural models and molecular simulations. <i>EPJ Web of Conferences</i> , 2012, 33, 02002.	0.1	9
40	A Solid State Density Functional Study of Crystalline Thiophene-Based Oligomers and Polymers. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14504-14509.	1.2	27
41	Molecular dynamics simulations of the solvent- and thermal history-dependent structure of the PCBM fullerene derivative. <i>Journal of Materials Chemistry</i> , 2012, 22, 5434.	6.7	29
42	Organic Peracids: A Structural Puzzle for ¹⁷ O NMR and Ab Initio Chemical Shift Calculations. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1814-1819.	1.1	13
43	Molecular dynamics simulation of rupture in glassy polymer bridges within filler aggregates. <i>Physical Review E</i> , 2012, 86, 041801.	0.8	22
44	Coarse-grained kinetic modelling of bilayer heterojunction organic solar cells. <i>Organic Electronics</i> , 2012, 13, 750-761.	1.4	13
45	Nonequilibrium simulations of filled polymer networks: Searching for the origins of reinforcement and nonlinearity. <i>Journal of Chemical Physics</i> , 2011, 134, 054902.	1.2	50
46	Coarse-Grained Simulations of Model Polymer Nanofibres. <i>Macromolecular Theory and Simulations</i> , 2011, 20, 305-319.	0.6	26
47	Molecular Modeling of Crystalline Alkylthiophene Oligomers and Polymers. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1591-1602.	1.2	87
48	Methodological assessment of kinetic Monte Carlo simulations of organic photovoltaic devices: The treatment of electrostatic interactions. <i>Journal of Chemical Physics</i> , 2010, 132, 094705.	1.2	74
49	Blending ionic liquids: how physico-chemical properties change. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1784.	1.3	69
50	Form II Poly(3-butylthiophene): Crystal Structure and Preferred Orientation in Spherulitic Thin Films. <i>Macromolecules</i> , 2010, 43, 6772-6781.	2.2	43
51	Ordered Stacking of Regioregular Head-to-Tail Polyalkylthiophenes: Insights from the Crystal Structure of Form I ϵ^2 Poly(3- <i>n</i> -butylthiophene). <i>Chemistry of Materials</i> , 2009, 21, 78-87.	3.2	50
52	Structural Organization and Transport Properties of Novel Pyrrolidinium-Based Ionic Liquids with Perfluoroalkyl Sulfonylimide Anions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10750-10759.	1.2	102
53	Theories and simulations of polymer-based nanocomposites: From chain statistics to reinforcement. <i>Progress in Polymer Science</i> , 2008, 33, 683-731.	11.8	256
54	Interaction of Water with the Model Ionic Liquid [bmim][BF ₄]: Molecular Dynamics Simulations and Comparison with NMR Data. <i>Journal of Physical Chemistry B</i> , 2008, 112, 7826-7836.	1.2	231

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73	Molecular Modeling of Crystalline Oligothiophenes: Testing and Development of Improved Force Fields. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18053-18064.	1.2	69
74	Computational reinvestigation of the bithiophene torsion potential. <i>Chemical Physics Letters</i> , 2003, 379, 364-372.	1.2	121
75	Application of the Christensen-Lo Model to the Reinforcement of Elastomers by Fractal Fillers. <i>Macromolecular Theory and Simulations</i> , 2003, 12, 17-23.	0.6	33
76	Side-Chain Role in Chemically Sensing Conducting Polymer Field-Effect Transistors. <i>Journal of Physical Chemistry B</i> , 2003, 107, 7589-7594.	1.2	101
77	Polymer-mediated adhesion: A statistical approach. <i>Journal of Chemical Physics</i> , 2003, 119, 9295-9307.	1.2	6
78	Confined polymer networks: The harmonic approach. <i>Journal of Chemical Physics</i> , 2002, 116, 3109-3118.	1.2	6
79	Degrees of Chirality in Helical Structures. <i>Macromolecular Theory and Simulations</i> , 2002, 11, 739-750.	0.6	13
80	Substituent effects on the second-order hyperpolarisability of cyanine cations. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 439-445.	1.5	3
81	Rigid filler particles in a rubber matrix: effective force constants by multipolar expansion. <i>Computational and Theoretical Polymer Science</i> , 2000, 10, 149-157.	1.1	9
82	Mesoscopic bead-and-spring model of hard spherical particles in a rubber matrix. I. Hydrodynamic reinforcement. <i>Journal of Chemical Physics</i> , 2000, 113, 7554-7563.	1.2	18
83	Halogen Bonding in Fluoroalkylhalides: A Quantum Chemical Study of Increasing Fluorine Substitution. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1617-1620.	1.1	198
84	Rotational barriers of amides and polyisocyanates: A spin-coupled study. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 249-258.	1.0	6
85	Polymer association in poor solvents: from monomolecular micelles to clusters of chains and phase separation. <i>Macromolecular Theory and Simulations</i> , 1999, 8, 65-84.	0.6	18
86	Rigid particles in an elastic polymer network: An electrical-analog approach. <i>Journal of Chemical Physics</i> , 1998, 109, 3285-3292.	1.2	6
87	Antiferromagnetic Spin Couplings in Cyclobutadiene Chains. <i>Journal of Physical Chemistry B</i> , 1997, 101, 6688-6691.	1.2	14
88	Macromolecular clusters in poor-solvent polymer solutions. <i>Journal of Chemical Physics</i> , 1997, 107, 6479-6490.	1.2	39
89	Spin-Coupled Valence Bond Study of the Reaction between Benzene and a Methyl Cation. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2886-2892.	1.1	16
90	Chain Interactions in Poor-Solvent Polymer Solutions: Equilibrium and Nonequilibrium Aspects. <i>Macromolecules</i> , 1996, 29, 6663-6670.	2.2	13

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91	A Cluster of Chains Can Be Smaller Than a Single Chain: A New Interpretation of Kinetics of Collapse Experiments. <i>Macromolecules</i> , 1996, 29, 8565-8567.	2.2	24
92	Rubber elasticity: A contact probability model with harmonic entanglement constraints. <i>Journal of Chemical Physics</i> , 1996, 105, 8352-8361.	1.2	2
93	Pair populations and effective valencies from ab initio SCF and spin-coupled wave functions. <i>International Journal of Quantum Chemistry</i> , 1996, 57, 501-518.	1.0	36
94	Chain collapse and phase separation in poor solvent polymer solutions: A unified molecular description. <i>Journal of Chemical Physics</i> , 1996, 104, 1626-1645.	1.2	54
95	Aromatic electrophilic substitution. A modern valence bond study. <i>Journal of the Chemical Society, Faraday Transactions</i> , 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. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 749.	1.7	7
97	The collapse of chains with different architectures. <i>Journal of Chemical Physics</i> , 1994, 100, 7804-7813.	1.2	17
98	Spin correlation in π -electron systems from spin-coupled wavefunctions. II. Further applications. <i>Chemical Physics</i> , 1994, 186, 251-273.	0.9	13
99	Spin correlation in π -electron systems from spin-coupled wavefunctions. I. Theory and first applications. <i>Chemical Physics</i> , 1994, 186, 233-250.	0.9	19
100	Spin-Coupled Study of the Electronic Structure of Polyenyl Radicals C ₃ H ₅ -C ₉ H ₁₁ . <i>Journal of the American Chemical Society</i> , 1994, 116, 2075-2084.	6.6	18
101	On the role of different spin bases within spin-coupled theory. <i>Molecular Physics</i> , 1993, 79, 197-216.	0.8	29
102	The Lowest Singlet and Triplet States of σ -Benzynes: Spin-Coupled Interpretation of the Electronic Structure at CAS SCF Equilibrium Geometries. <i>Israel Journal of Chemistry</i> , 1993, 33, 253-264.	1.0	27
103	Fracture in Silica/Butadiene Rubber: A Molecular Dynamics View of Design-Property Relationships. <i>ACS Polymers Au</i> , 0, , .	1.7	9