Mesfin Tsige

List of Publications by Year
in descending order

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72 papers	1,707 citations	331670 21 h-index	315739 38 g-index
72 all docs	72 docs citations	72 times ranked	2585 citing authors

#	Article	IF	Citations
1	Single-Junction Polymer Solar Cells with Over 10% Efficiency by a Novel Two-Dimensional Donorâ€“Acceptor Conjugated Copolymer. ACS Applied Materials & Interfaces, 2015, 7, 4928-4935.	8.0	256
2	Atomistic Simulations of End-Linked Poly(dimethylsiloxane) Networks:Â Structure and Relaxation. Macromolecules, 2004, 37, 3857-3864.	4.8	135
3	Molecular Modeling Approach to Prediction of Thermo-Mechanical Behavior of Thermoset Polymer Networks. Macromolecules, 2012, 45, 5307-5315.	4.8	132
4	Interfacial Structure and Dynamics of Siloxane Systems: PDMSâ^'Vapor and PDMSâ^'Water. Macromolecules, 2009, 42, 3186-3194.	4.8	74
5	Molecular dynamics simulation of solventâ€“polymer interdiffusion: Fickian diffusion. Journal of Chemical Physics, 2004, 120, 2989-2995.	3.0	57
6	Molecular modeling of elastic properties of thermosetting polymers using aÂdynamic deformation approach. Polymer, 2013, 54, 3370-3376.	3.8	53
7	Improved Force Field for Molecular Modeling of Poly(3-hexylthiophene). Journal of Physical Chemistry B, 2013, 117, 10035-10045.	2.6	52
8	Chain length and torsional dependence of exciton binding energies in P3HT and PTB7 conjugated polymers: A first-principles study. Polymer, 2014, 55, 2667-2672.	3.8	52
9	Surface tension of normal and branched alkanes. Molecular Physics, 2007, 105, 3155-3163.	1.7	45
10	Molecular Structure of Poly(methyl methacrylate) Surface. I. Combination of Interface-Sensitive Infraredâ€“Visible Sum Frequency Generation, Molecular Dynamics Simulations, and ab Initio Calculations. Langmuir, 2014, 30, 11609-11618.	3.5	44
11	Thermal Properties and Segmental Dynamics of Polymer Melt Chains Adsorbed on Solid Surfaces. Langmuir, 2018, 34, 4199-4209.	3.5	43
12	Conformations and torsional potentials of poly(3-hexylthiophene) oligomers: Density functional calculations up to the dodecamer. Computational and Theoretical Chemistry, 2012, 995, 36-42.	2.5	37
13	Surface Tension and Surface Orientation of Perfluorinated Alkanes. Journal of Physical Chemistry C, 2008, 112, 5029-5035.	3.1	31
14	Polymers Based on Benzodipyrrolidone and Naphthodipyrrolidone with Latent Hydrogenâ€Bonding on the Main Chain. Macromolecular Chemistry and Physics, 2017, 218, 1600617.	2.2	30
15	Structural properties of atactic polystyrene adsorbed onto solid surfaces. Journal of Chemical Physics, 2011, 135, 174708.	3.0	28
16	Elucidating the Origin of the Attractive Force among Hydrophilic Macroions. Scientific Reports, 2016, 6, 26595.	3.3	27
17	Molecular Structure of Poly(methyl methacrylate) Surface II: Effect of Stereoregularity Examined through All-Atom Molecular Dynamics. Langmuir, 2014, 30, 12775-12785.	3.5	25
18	Application of Carbon Nanotubes for Removing Organic Contaminants from Water. Materials Express, 2011, 1, 183-200.	0.5	24

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19	Morphology of Evaporated Multiblock Copolymer Membranes Studied by Molecular Dynamics Simulations. Macromolecules, 2004, 37, 9132-9138.	4.8	23
20	Nanostructures and Electronic Properties of a High-Efficiency Electron-Donating Polymer. Journal of Physical Chemistry A, 2013, 117, 12628-12634.	2.5	23
21	On Modulating Interfacial Structure towards Improved Anti-Icing Performance. Coatings, 2016, 6, 3.	2.6	22
22	Structure of Poly(dialkylsiloxane) Melts:â€‰ Comparisons of Wide-Angle X-ray Scattering, Molecular Dynamics Simulations, and Integral Equation Theory. Macromolecules, 2007, 40, 7036-7043.	4.8	20
23	Continuous Curvature Change into Controllable and Responsive Onion-like Vesicles by Rigid Sphereâ€“Rod Amphiphiles. ACS Nano, 2020, 14, 1811-1822.	14.6	20
24	Chain Network: Key to the Ductile Behavior of Polymer Glasses. Macromolecules, 2018, 51, 1666-1673.	4.8	19
25	Tuning range-separated DFT functionals for accurate orbital energy modeling of conjugated molecules. Computational and Theoretical Chemistry, 2015, 1070, 14-20.	2.5	18
26	Effect of tacticity on the structure and glass transition temperature of polystyrene adsorbed onto solid surfaces. Journal of Chemical Physics, 2018, 148, 134705.	3.0	18
27	Interfacial Properties of Oxidized Polystyrene and Its Interaction with Water. Langmuir, 2013, 29, 13230-13238.	3.5	17
28	Interfacial properties of free-standing poly(3-hexylthiophene) films. Journal of Chemical Physics, 2012, 137, 044703.	3.0	16
29	MOLECULAR MODELING OF THERMAL AND MECHANICAL PROPERTIES OF ELASTOMERS: A REVIEW. Rubber Chemistry and Technology, 2013, 86, 401-422.	1.2	16
30	Surface enrichment driven by polymer topology. Physical Review E, 2016, 93, 050501.	2.1	16
31	Characterizing the Hydrophobicity of Surfaces Using the Dynamics of Interfacial Water Molecules. Journal of Physical Chemistry C, 2018, 122, 9015-9020.	3.1	14
32	Unique Symmetry-Breaking Phenomenon during the Self-assembly of Macroions Elucidated by Simulation. Scientific Reports, 2018, 8, 13076.	3.3	14
33	Static and dynamic properties of poly(3-hexylthiophene) films at liquid/vacuum interfaces. Journal of Chemical Physics, 2012, 137, 204701.	3.0	13
34	Effect of Fluorination on Electronic Properties of Polythienothiophene-co-benzodithiophenes and Their Fullerene Complexes. ACS Applied Materials & Interfaces, 2014, 6, 15889-15896.	8.0	13
35	Probing calcium solvation by XAS, MD and DFT calculations. RSC Advances, 2020, 10, 27315-27321.	3.6	12
36	Cooperative Multivalent Weak and Strong Interfacial Interactions Enhance the Adhesion of Mussel-Inspired Adhesives. Macromolecules, 2021, 54, 5417-5428.	4.8	12

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37	Toward the Rational Design of Organic Solar Photovoltaics: Application of Molecular Structure Methods to Donor Polymers. Journal of Physical Chemistry A, 2021, 125, 10593-10603.	2.5	12
38	Packing of poly(tetrafluoroethylene) in the liquid state: Molecular dynamics simulation and theory. Journal of Chemical Physics, 2008, 129, 214901.	3.0	11
39	Carbon nanotube-textured sand for controlling bioavailability of contaminated sediments. Nano Research, 2010, 3, 412-422.	10.4	11
40	Torsionally-Induced Blue Shift of the Band Gap in Poly(3-Hexylthiophene). Journal of Computational and Theoretical Nanoscience, 2014, 11, 2157-2164.	0.4	11
41	Local Structure Contributions to Surface Tension of a Stereoregular Polymer. ACS Macro Letters, 2015, 4, 1234-1238.	4.8	11
42	Understanding the effect of heteroatoms on structural and electronic properties of conjugated polymers. Polymer, 2015, 56, 293-299.	3.8	11
43	Carbon Nanotube Based Groundwater Remediation: The Case of Trichloroethylene. Molecules, 2016, 21, 953.	3.8	11
44	Effect of Polymer/Solid and Polymer/Vapor Instantaneous Interfaces on the Interfacial Structure and Dynamics of Polymer Melt Systems. Langmuir, 2016, 32, 7151-7158.	3.5	11
45	Molecular Dynamics Simulation Study of Polymer Nanocomposites with Controllable Dispersion of Spherical Nanoparticles. Journal of Physical Chemistry B, 2017, 121, 10146-10156.	2.6	11
46	Strain rate and temperature dependence of the mechanical properties of polymers: A universal time-temperature superposition principle. Journal of Chemical Physics, 2018, 149, 044105.	3.0	11
47	Proximity to Graphene Dramatically Alters Polymer Dynamics. Macromolecules, 2019, 52, 5074-5085.	4.8	11
48	Co-ion Effects in the Self-Assembly of Macroions: From Co-ions to Co-macroions and to the Unique Feature of Self-Recognition. Langmuir, 2020, 36, 10519-10527.	3.5	11
49	Solvent and Substrate Induced Synergistic Ordering in Block Copolymer Thin Films. Macromolecules, 2018, 51, 7186-7196.	4.8	9
50	Atomistic Insights into Hydrogen-Bonding-Driven Competitive Adsorption of Acetoneâ€“Chloroform Binary Mixtures. Journal of Physical Chemistry C, 2019, 123, 29729-29738.	3.1	9
51	Simulation Study of the Silicon Oxide and Water Interface. Journal of Computational and Theoretical Nanoscience, 2010, 7, 2586-2601.	0.4	8
52	Epitaxial transfer through end-group coordination modulates the oddâ€“even effect in an alkanethiol monolayer assembly. Nanoscale, 2014, 6, 3496-3502.	5.6	8
53	Understanding structural and electronic properties of dithienyl benzothiadiazole and its complex with C70. Polymer, 2015, 75, 73-77.	3.8	8
54	Spreading Dynamics of Water Droplets on a Completely Wetting Surface. Journal of Physical Chemistry C, 2020, 124, 20109-20115.	3.1	8

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55	High Adsorption of Benzoic Acid on Single Walled Carbon Nanotube Bundles. Scientific Reports, 2020, 10, 10013.	3.3	8
56	Interfacial and wetting properties of poly(3-hexylthiophene)â€“water systems. Chemical Physics Letters, 2015, 635, 139-145.	2.6	7
57	Synthesis and Characterization of Well-Defined, Tadpole-Shaped Polystyrene with a Single Atom Junction Point. Macromolecules, 2018, 51, 9509-9518.	4.8	7
58	Interaction Geometry Causes Spectral Line-Shape Broadening at the Solid/Liquid Interface. Journal of Physical Chemistry C, 2019, 123, 30447-30457.	3.1	7
59	Adsorption of aromatic carboxylic acids on carbon nanotubes: impact of surface functionalization, molecular size and structure. Environmental Sciences: Processes and Impacts, 2019, 21, 2109-2117.	3.5	6
60	Structure and Dynamics of Nanoconfined Water Between Surfactant Monolayers. Langmuir, 2020, 36, 447-455.	3.5	6
61	Tuning Solvent Quality Induces Morphological Phase Transitions in Miktoarm Star Polymer Films. Macromolecules, 2020, 53, 6151-6162.	4.8	6
62	Hydrogen bond directed surface dynamics at tactic poly(methyl methacrylate)/water interface. Soft Matter, 2017, 13, 8556-8564.	2.7	5
63	Surface Segregation of Cyclic Chains in Binary Melts of Thin Polymer Films: The Influence of Constituent Concentration. Polymers, 2018, 10, 324.	4.5	5
64	Effect of chain stiffness on the morphology of diblock copolymer melts. Journal of Polymer Science, Part B: Polymer Physics, 2009, 47, 2556-2565.	2.1	4
65	Interfacial Engineering for Oil and Gas Applications: Role of Modeling and Simulation. , 2016, , 257-283.		3
66	Understanding the origin of structure sensitivity in hydrodechlorination of trichloroethylene on a palladium catalyst. Reaction Chemistry and Engineering, 2021, 6, 2270-2279.	3.7	3
67	Adsorption of Benzoic Acid: Structural Organization on the Surfaces of Pristine and Functionalized Single-Walled Carbon Nanotubes. ACS ES&T Water, 2021, 1, 251-258.	4.6	2
68	Single Chain Hydration and Dynamics of Mussel-Inspired Soybean-Based Adhesive. Jom, 2021, 73, 2460-2470.	1.9	2
69	Rational Control of Selfâ€Recognition of Macroionic Î³â€Cyclodextrin by Hostâ€Guest Interaction with Superâ€Chaotropic Borate Cluster Ions. ChemPlusChem, 2020, 85, 2316-2319.	2.8	1
70	Adsorptive Structure and Mobility on Carbon Nanotube Exteriors Using Benzoic Acid as a Molecular Probe of Amphiphilic Water Contaminants. Journal of Physical Chemistry B, 0, , .	2.6	1
71	Soft Templating of Water Aggregates Disrupts Ï€â€“Ï€ Stacking in Crystalline Poly(3-hexylthiophene). Journal of Physical Chemistry C, 2018, 122, 422-428.	3.1	0
72	Phase manipulation of topologically engineered AB-type multi-block copolymers. RSC Advances, 2019, 9, 42029-42042.	3.6	0