## Germano Heinzelmann

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Position of the Third Na+ Site in the Aspartate Transporter GltPh and the Human Glutamate Transporter, EAAT1. PLoS ONE, 2012, 7, e33058.	1.1	65
2	A Potent and Selective Peptide Blocker of the Kv1.3 Channel: Prediction from Free-Energy Simulations and Experimental Confirmation. PLoS ONE, 2013, 8, e78712.	1.1	58
3	Automation of absolute protein-ligand binding free energy calculations for docking refinement and compound evaluation. Scientific Reports, 2021, 11, 1116.	1.6	49
4	Attach-Pull-Release Calculations of Ligand Binding and Conformational Changes on the First BRD4 Bromodomain. Journal of Chemical Theory and Computation, 2017, 13, 3260-3275.	2.3	49
5	Amphiphilic polyurethane hydrogels as smart carriers for acidic hydrophobic drugs. International Journal of Pharmaceutics, 2018, 546, 106-114.	2.6	39
6	Electrospun nanofibrous scaffolds of segmented polyurethanes based on PEG, PLLA and PTMC blocks: Physico-chemical properties and morphology. Materials Science and Engineering C, 2015, 56, 511-517.	3.8	36
7	Free Energy Simulations of Ligand Binding to the Aspartate Transporter GltPh. Biophysical Journal, 2011, 101, 2380-2388.	0.2	32
8	Computation of Standard Binding Free Energies of Polar and Charged Ligands to the Glutamate Receptor GluA2. Journal of Physical Chemistry B, 2014, 118, 1813-1824.	1.2	27
9	Mechanism and Energetics of Ligand Release in the Aspartate Transporter Glt <sub>Ph</sub> . Journal of Physical Chemistry B, 2013, 117, 5486-5496.	1.2	26
10	Thermoâ€responsive polyurethane hydrogels based on poly(ethylene glycol) and poly(caprolactone): Physicoâ€chemical and mechanical properties. Journal of Applied Polymer Science, 2016, 133, .	1.3	26
11	Plasticization of Poly(3-hydroxybutyrate- <i>co</i> -3-hydroxyvalerate) with an Oligomeric Polyester: Miscibility and Effect of the Microstructure and Plasticizer Distribution on Thermal and Mechanical Properties. ACS Omega, 2021, 6, 3278-3290.	1.6	24
12	Confined PEO crystallisation in immiscible PEO/PLLA blends. RSC Advances, 2016, 6, 30937-30950.	1.7	22
13	Na+ Interactions with the Neutral Amino Acid Transporter ASCT1. Journal of Biological Chemistry, 2014, 289, 17468-17479.	1.6	21
14	Rice husk/poly(propyleneâ€ <i>co</i> â€ethylene) composites: Effect of different coupling agents on mechanical, thermal, and morphological properties. Journal of Applied Polymer Science, 2012, 123, 3337-3344.	1.3	19
15	Molecular Dynamics Simulations of the Mammalian Glutamate Transporter EAAT3. PLoS ONE, 2014, 9, e92089.	1.1	18
16	Enzymatic synthesis and structural characterization of methacryloylâ€Dâ€fructose―and methacryloylâ€Dâ€glucoseâ€based monomers and poly(methacryloylâ€Dâ€fructose)â€based hydrogels. Journal o Chemical Technology and Biotechnology, 2018, 93, 1694-1704.	of1.6	16
17	Preparation and characterization of cellulose acetate/polysiloxane composites. Cellulose, 2013, 20, 2791-2802.	2.4	15
18	Plasticization of poly(3â€hydroxybutyrate) with triethyl citrate: Thermal and mechanical properties, morphology, and kinetics of crystallization. Journal of Applied Polymer Science, 2021, 138, 49990.	1.3	14

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19	Molecular Dynamics Simulations Elucidate the Mechanism of Proton Transport in the Glutamate Transporter EAAT3. Biophysical Journal, 2014, 106, 2675-2683.	0.2	13
20	Effect of diisocyanates and chain extenders on the physicochemical properties and morphology of multicomponent segmented polyurethanes based on poly(l -lactide), poly(ethylene glycol) and poly(trimethylene carbonate). Polymer International, 2015, 64, 1326-1335.	1.6	13
21	Thermoresponsive hydrogels based on sucrose 1â€ <i>O</i> ′â€methacrylate and <i>N</i> â€isopropylacrylamide: Synthesis, properties, and applications. Journal of Applied Polymer Science, 2017, 134, 45495.	1.3	12
22	Colloidal Behavior of Cellulose Nanocrystals Grafted with Poly(2-alkyl-2-oxazoline)s. ACS Omega, 2019, 4, 11893-11905.	1.6	12
23	Influence of the synthesis conditions on the structural and thermal properties of poly( <scp>l</scp> â€lactide)â€ <i>b</i> â€poly(ethylene glycol)â€ <i>b</i> â€poly( <scp>l</scp> â€lactide). Journal o Applied Polymer Science, 2014, 131, .	of1.3	10
24	A one-pot, solvent-free, and controlled synthetic route for thermoresponsive hyperbranched polyurethanes. Polymer Chemistry, 2020, 11, 6295-6307.	1.9	10
25	Sucrose Methacrylate-Based Amphiphilic Block Copolymers. Macromolecular Chemistry and Physics, 2017, 218, 1600452.	1.1	9
26	Monte Carlo simulations for amphiphilic aggregation near a water phase transition. Journal of Chemical Physics, 2009, 131, 144901.	1.2	8
27	Structures and morphologies of <i>in situ</i> polymerized blends of PMMA and ASA. Journal of Applied Polymer Science, 2013, 130, 654-664.	1.3	7
28	pH and thermo-responsive hybrid hydrogels based on PNIPAAM and keratin. European Polymer Journal, 2020, 125, 109538.	2.6	7
29	Micellar dynamics and water–water hydrogen-bonding from temperature-jump Monte Carlo simulations. Chemical Physics Letters, 2012, 550, 83-87.	1.2	6
30	Computational Studies of Glutamate Transporters. Biomolecules, 2015, 5, 3067-3086.	1.8	6
31	Calculation of free energy changes due to mutations from alchemical free energy simulations. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550023.	1.8	6
32	Mechanism and Kinetics of Lipase-Catalyzed Polycondensation of Glycerol and Sebacic Acid: Influence of Solvent and Temperature. Biomacromolecules, 2022, 23, 2968-2975.	2.6	6
33	Interplay between micelle formation and waterlike phase transitions. Journal of Chemical Physics, 2010, 132, 064905.	1.2	5
34	Morphology and mechanical properties of nanocomposites of cellulose acetate and organic montmorillonite prepared with different plasticizers. Journal of Applied Polymer Science, 2012, 124, 4628-4635.	1.3	5
35	Orientational dynamics for an amphiphilic-solvent solution. Journal of Chemical Physics, 2011, 134, 064901.	1.2	5
36	The influence of rigid and flexible monomers on the physical hemical properties of polyimides. Journal of Applied Polymer Science, 2014, 131, .	1.3	5

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37	Telechelic Poly(bisphenol A carbonate) Synthesis by Glycolysis: A Response Surface Methodology Approach. Industrial & Engineering Chemistry Research, 2017, 56, 3983-3992.	1.8	5
38	Triblock Copolymers Based on Sucrose Methacrylate and Methyl Methacrylate: RAFT Polymerization and Selfâ€Assembly. Macromolecular Chemistry and Physics, 2020, 221, 1900561.	1.1	5
39	Effect of <i>in situ</i> polymerization conditions of methyl methacrylate on the structural and morphological properties of poly(methyl) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 662 Td (methacrylate)/pd	oly(acrylor	nitrileâ€ <i>g&lt;</i>
40	PMMA/AES Blends, fournal of Applied Polymer Science, 2012, 124, 2846-2856. Self-assembly of dual-responsive amphiphilic POEGMA- <i>b</i> -P4VP- <i>b</i> -POEGMA triblock copolymers: effect of temperature, pH, and complexation with Cu <sup>2+</sup> . Polymer Chemistry, 2021, 12, 4668-4679.	1.9	4
41	Combining CROP and ATRP to synthesize pH-responsive poly(2-ethyl-2-oxazoline- <i>b</i> -4-vinylpyridine) block copolymers. Polymer Chemistry, 2021, 12, 4680-4695.	1.9	4
42	Dynamics of micelle formation from temperature-jump Monte Carlo simulations. Physical Review E, 2015, 92, 052305.	0.8	3
43	Macroporous hydrogels based on carbohydrates monomethacrylates and dimethacrylates: singular properties from carbohydrateâ€based crosslinkers. Journal of Chemical Technology and Biotechnology, 2019, 94, 1913-1924.	1.6	3
44	Shedding Light on the Hydrolysis Mechanism of cis, trans-[Ru(dmso) <sub>4</sub> Cl <sub>2</sub> ] Complexes and Their Interactions with DNA—A Computational Perspective. Journal of Physical Chemistry B, 2019, 123, 457-467.	1.2	3
45	A theoretical investigation on the aminolysis of pyromellitic and 1,4,5,8-naphthalenetetracarboxylic dianhydrides. Computational and Theoretical Chemistry, 2019, 1147, 13-19.	1.1	1
46	Twoâ€step route polycondensation for polynaphthalimides synthesis through high molar mass soluble precursors: A kinetic study. Journal of Applied Polymer Science, 2020, 137, 49262.	1.3	1
47	Stimuliâ€Responsive Hydrogels Based on Random Copolymers of the Sucrose Methacrylate. Macromolecular Materials and Engineering, 0, , 2100378.	1.7	1
48	Insights into the Human Glutamate Transporters from the Bacterial Homolog Glt(Ph). Biophysical Journal, 2013, 104, 109a.	0.2	0