Igor M Neelov

List of Publications by Year in Descending Order

77 papers	1,179 citations	24 h-index	31 g-index
80 ext. papers	1,286 ext. citations	3.3 avg, IF	4.23 L-index

#	Paper	IF	Citations
77	Thermoresponsive Molecular Brushes with a Rigid-Chain Aromatic Polyester Backbone and Poly-2-alkyl-2-oxazoline Side Chains. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
76	Size and Structure of Empty and Filled Nanocontainer Based on Peptide Dendrimer with Histidine Spacers at Different pH. *Molecules*, **2021**, 26,	4.8	2
75	Poly(lysine) Dendrimers Form Complexes with siRNA and Provide Its Efficient Uptake by Myeloid Cells: Model Studies for Therapeutic Nucleic Acid Delivery. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	25
74	Why the Orientational Mobility in Arginine and Lysine Spacers of Peptide Dendrimers Designed for Gene Delivery Is Different?. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	3
73	Application of new lysine-based peptide dendrimers D3K2 and D3G2 for gene delivery: Specific cytotoxicity to cancer cells and transfection in vitro. *Bioorganic Chemistry*, **2020**, 95, 103504	5.1	31
72	Comparison of Structure and Local Dynamics of Two Peptide Dendrimers with the Same Backbone but with Different Side Groups in Their Spacers. *Polymers*, **2020**, 12,	4.5	5
71	Molecular Dynamics and Spin-Lattice NMR Relaxation in (alpha)- and (varepsilon)-Polylysine. *Applied Magnetic Resonance*, **2020**, 51, 1669-1679	0.8	2
70	SCF Theory of Uniformly Charged Dendrimers: Impact of Asymmetry of Branching, Generation Number, and Salt Concentration. *Macromolecules*, **2020**, 53, 7298-7311	5.5	6
69	Stable Deuterium Labeling of Histidine-Rich Lysine-Based Dendrimers. *Molecules*, **2019**, 24,	4.8	13
68	Lysine-based dendrimer with double arginine residues.. *RSC Advances*, **2019**, 9, 18018-18026	3.7	16
67	Computer simulation of complex of lysine dendrigraft with molecules of therapeutic KED peptide. *ITM Web of Conferences*, **2019**, 24, 02008	0.1	
66	Self-Assembly of Lysine-Based Dendritic Surfactants Modeled by the Self-Consistent Field Approach. *Langmuir*, **2018**, 34, 1613-1626	4	18
65	Structure and properties of polydisperse polyelectrolyte brushes studied by self-consistent field theory. *Soft Matter*, **2018**, 14, 6230-6242	3.6	11
64	Effect of an asymmetry of branching on structural characteristics of dendrimers revealed by Brownian dynamics simulations. *Polymer*, **2018**, 146, 256-266	3.9	12
63	Complexes and conjugates of lysine dendrimer with therapeutic tetrapeptides. Molecular dynamics simulation **2018**,		1
62	Lysine Dendrigraft Nanocontainers. Influence of Topology on Their Size and Internal Structure. *Pharmaceutics*, **2018**, 10,	6.4	9
61	NMR studies of excluded volume interactions in peptide dendrimers. *Scientific Reports*, **2018**, 8, 8916	4.9	19

60	Lysine Dendrimers and Their Complexes with Therapeutic and Amyloid Peptides: Computer Simulation **2018**,		2
59	Planar Brush of End-Tethered Molecular Bottle-Brushes. Scaling Mode. *Polymer Science - Series C*, **2018**, 60, 76-83	1.1	3
58	Nonexponential Kinetics of Loop Formation in Proteins and Peptides: A Signature of Rugged Free Energy Landscapes?. *Journal of Physical Chemistry B*, **2017**, 121, 9518-9525	3.4	22
57	Structure of asymmetrical peptide dendrimers: Insights given by self-consistent field theory. *Polymer*, **2017**, 125, 292-302	3.9	19
56	Interaction of Lysine Dendrigraft of 2nd Generation and Semax Peptide. Molecular Dynamics Simulation **2017**,		1
55	Is the manifestation of the local dynamics in the spin-lattice NMR relaxation in dendrimers sensitive to excluded volume interactions?. *Physical Chemistry Chemical Physics*, **2016**, 18, 24307-17	3.6	24
54	Molecular Dynamics Simulation of Lysine Dendrimer and Oppositely Charged Semax Peptides **2016**,		1
53	Molecular Dynamics Simulation of Interaction of Short Lysine Brush and Oppositely Charged Semax Peptides. *Natural Science*, **2016**, 08, 499-510	0.5	2
52	Molecular dynamics simulation of spin-lattice NMR relaxation in poly-L-lysine dendrimers: manifestation of the semiflexibility effect. *Physical Chemistry Chemical Physics*, **2015**, 17, 3214-26	3.6	41
51	Wet spinning of fibers made of chitosan and chitin nanofibrils. *Carbohydrate Polymers*, **2014**, 108, 176-82	10.3	88
50	Mathematical simulation of lysine dendrimers: Temperature dependences. *Polymer Science - Series C*, **2013**, 55, 154-161	1.1	24
49	Are structural properties of dendrimers sensitive to the symmetry of branching? Computer simulation of lysine dendrimers. *Journal of Chemical Physics*, **2013**, 139, 064903	3.9	37
48	Molecular properties of lysine dendrimers and their interactions with A□peptides and neuronal cells. *Current Medicinal Chemistry*, **2013**, 20, 134-43	4.3	10
47	Mechanism of shear deformation of a coiled myosin coil: Computer simulation. *Polymer Science - Series A*, **2010**, 52, 662-670	1.2	7
46	The theory of viscoelastic characteristics of a highly stretched macromolecule in single molecule AFM. *Polymer Science - Series A*, **2009**, 51, 940-956	1.2	2
45	Simulation of the Mechanical Unfolding of the Ubiquitin by Pulling in Different Directions with Constant Speed. *Macromolecular Symposia*, **2009**, 278, 105-113	0.8	2
44	Molecular Dynamics of Pectin Extension. *Macromolecular Symposia*, **2007**, 252, 140-148	0.8	4
43	Molecular dynamics simulation of dextran extension by constant force in single molecule AFM. *Biophysical Journal*, **2006**, 91, 3579-88	2.9	26

42	Molecular Dynamic Simulation of Side-Chain Liquid Crystalline Elastomer. *Macromolecular Symposia*, **2006**, 237, 119-127	0.8	4
41	Molecular Dynamics Simulation of Dextran Extension at Constant Pulling Speed. *Macromolecular Symposia*, **2006**, 237, 81-89	0.8	4
40	New Molecular Mechanism of Dextran Extension in Single Molecule AFM. *Lecture Notes in Computer Science*, **2006**, 711-720	0.9	2
39	Modelling of gas transport properties of polymer electrolytes containing various amounts of water. *Polymer*, **2004**, 45, 4171-4179	3.9	14
38	Molecular dynamics simulation of a flexible polymer network in a liquid crystal solvent; structure and equilibrium properties. *Polymer*, **2004**, 45, 4857-4866	3.9	5
37	Molecular dynamics simulation of a flexible polymer network in a liquid crystalline solvent; dynamical properties. *Polymer*, **2004**, 45, 8901-8911	3.9	2
36	Brownian Dynamics Simulation of Hyperbranched Polymers under Elongational Flow. *Journal of Physical Chemistry B*, **2004**, 108, 7627-7636	3.4	32
35	Conformational mobility of carbosilane dendrimer: Molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2004**, 6, 1285	3.6	31
34	Computer simulations of stretching and collapse of polymer molecules in solution. *Macromolecular Symposia*, **2003**, 191, 41-50	0.8	1
33	Computer simulation of the liquid crystal formation in a semi-flexible polymer system. *Macromolecular Symposia*, **2003**, 191, 191-200	0.8	3
32	Brownian Dynamics Simulations of Dendrimers under Elongational Flow: Bead−Rod Model with Hydrodynamic Interactions. *Macromolecules*, **2003**, 36, 6914-6924	5.5	32
31	Anisotropy of diffusion in a liquid crystalline system of semi-flexible polymer chains. *Physical Chemistry Chemical Physics*, **2003**, 5, 2410-2416	3.6	11
30	Conformational variability of helix sense reversals in poly(methyl isocyanate). *Polymer*, **2002**, 43, 1527-1532	3.9	4
29	Brownian dynamics simulation of linear polymers under elongational flow: Bead−rod model with hydrodynamic interactions. *Journal of Chemical Physics*, **2002**, 117, 4030-4041	3.9	32
28	Computer simulations of hyperbranched polymers: The influence of the Wiener index on the intrinsic viscosity and radius of gyration. *Journal of Chemical Physics*, **2002**, 117, 7802-7812	3.9	50
27	Molecular Dynamics Simulations of Polymers of Unsubstituted and Substituted Poly(p-phenylene terephthalate)s in the Bulk State. *Macromolecular Theory and Simulations*, **2001**, 10, 137-143	1.5	1
26	Estimation of the ion conductivity of a PEO-based polyelectrolyte system by molecular modeling. *Polymer*, **2001**, 42, 8043-8050	3.9	33
25	Modeling of water-free and water containing solid polyelectrolytes. *Polymer*, **2000**, 41, 985-990	3.9	27

24	Simulation of a PEO based solid polyelectrolyte, comparison of the CMM and the Ewald summation method. *Polymer*, **2000**, 41, 2149-2155	3.9	24
23	Molecular dynamics simulation of the structure of PEO based solid polymer electrolytes. *Polymer*, **2000**, 41, 4057-4063	3.9	32
22	Molecular dynamics simulation of the PEO sulfonic acid anion in water. *Computational and Theoretical Polymer Science*, **2000**, 10, 403-410		25
21	Computer simulation of polymer brushes under shear. *Rheologica Acta*, **2000**, 39, 469-475	2.3	7
20	Theory of Electric Birefringence of Long Flexible Polymer Chains with Transverse Bond Dipole Moments:Tetrahedral Lattice Model. *Macromolecules*, **2000**, 33, 9126-9135	5.5	2
19	Conformational study of substituted p-phenylene terephthalates with molecular mechanics and Metropolis Monte Carlo methods. *Polymer*, **1999**, 40, 2313-2321	3.9	4
18	Free Volume and Tacticity in Polystyrenes. *Macromolecules*, **1999**, 32, 1930-1938	5.5	45
17	New conformations and new types of helix sense reversals and defects in the chains of nonchiral poly(alkyl isocyanates). *Macromolecular Symposia*, **1999**, 146, 251-257	0.8	1
16	Collapse of diblock copolymer in poor solvent. Molecular dynamics study. *Macromolecular Symposia* , **1999**, 146, 267-273	0.8	1
15	Stochastic dynamics simulation of grafted polymer brushes under shear deformation. *Macromolecular Theory and Simulations*, **1998**, 7, 141-156	1.5	35
14	A computer simulation of the molecular properties of amorphous poly(vinyl chloride), PVC. *Journal of Non-Crystalline Solids*, **1998**, 235-237, 340-345	3.9	8
13	Stochastic dynamics of polymer brushes under shear deformation. *Journal of Non-Crystalline Solids*, **1998**, 235-237, 731-736	3.9	4
12	Theory of Electric Birefringence in a Strong Field for a Long Flexible Polymer Chain: Tetrahedral Lattice Model. *Macromolecules*, **1998**, 31, 9354-9361	5.5	2
11	Molecular Dynamics Simulation of Main Chain Liquid Crystalline Polymers. *Macromolecules*, **1998**, 31, 4626-4634	5.5	56
10	Shear deformation of two interpenetrating polymer brushes: Stochastic dynamics simulation. *Journal of Chemical Physics*, **1998**, 108, 6973-6988	3.9	34
9	Brownian dynamics simulation of grafted polymer brushes. *Macromolecular Theory and Simulations*, **1995**, 4, 119-136	1.5	28
8	Brownian dynamics of grafted polymer chains: time dependent properties. *Macromolecular Theory and Simulations*, **1995**, 4, 1063-1084	1.5	24
7	Brownian dynamics of polymer chains in external fields of different symmetry. *Journal of Non-Crystalline Solids*, **1994**, 172-174, 794-796	3.9	1

6	Brownian dynamics of polymeric chain in strong external field. *Macromolecular Symposia*, **1994**, 81, 55-62	0.8	2
5	Anisotropy of local relaxation properties of macromolecules. Polarized luminescence. *Die Makromolekulare Chemie Theory and Simulations*, **1993**, 2, 1-11		3
4	Theoretical analysis of the processes of heat exchange and relaxation of a polymer melt at the formation of highly oriented polymer films. *Acta Polymerica*, **1991**, 42, 245-250		
3	Distribution of correlation times and relationships of nuclear magnetic relaxation (13C) and nuclear Overhauser effect. *Acta Polymerica*, **1989**, 40, 643-648		2
2	Properties of kinetic element and local mobility of polymer chains. *Acta Polymerica*, **1984**, 35, 124-129		21
1	Investigation of Local Motions in Polymers by the Method of Molecular Dynamics. *Macromolecules*, **1980**, 13, 602-608	5.5	40