Paola Carbone

List of Publications by Year
in descending order

90 papers	5,941 citations	185998 28 h-index	71532 76 g-index
93 all docs	93 docs citations	93 times ranked	7244 citing authors

#	Article	IF	Citations
1	Precise and Ultrafast Molecular Sieving Through Graphene Oxide Membranes. Science, 2014, 343, 752-754.	6.0	2,060
2	Tunable sieving of ions using graphene oxide membranes. Nature Nanotechnology, 2017, 12, 546-550.	15.6	1,364
3	Temperature-Transferable Coarse-Grained Potentials for Ethylbenzene, Polystyrene, and Their Mixtures. Macromolecules, 2008, 41, 9919-9929.	2.2	210
4	Transferability of coarse-grained force fields: The polymer case. Journal of Chemical Physics, 2008, 128, 064904.	1.2	192
5	Van der Waals pressure and its effect on trapped interlayer molecules. Nature Communications, 2016, 7, 12168.	5.8	137
6	How Good Are Coarseâ€Grained Polymer Models? A Comparison for Atactic Polystyrene. ChemPhysChem, 2012, 13, 3428-3439.	1.0	100
7	Coarse-Graining Poly(ethylene oxide)â€“Poly(propylene oxide)â€“Poly(ethylene oxide) (PEOâ€“PPOâ€“PEO) Block Copolymers Using the MARTINI Force Field. Journal of Physical Chemistry B, 2014, 118, 1648-1659.	1.2	69
8	IBIsCO: A molecular dynamics simulation package for coarseâ€grained simulation. Journal of Computational Chemistry, 2011, 32, 1475-1487.	1.5	68
9	A multiscale approach to model hydrogen bonding: The case of polyamide. Journal of Chemical Physics, 2015, 142, 224907.	1.2	68
10	Studying long-time dynamics of imidazolium-based ionic liquids with a systematically coarse-grained model. Physical Chemistry Chemical Physics, 2010, 12, 4714.	1.3	65
11	Effective Polarization in Pairwise Potentials at the Grapheneâ€“Electrolyte Interface. Journal of Physical Chemistry Letters, 2017, 8, 703-708.	2.1	62
12	Interactions of PEOâ€“PPOâ€“PEO block copolymers with lipid membranes: a computational and experimental study linking membrane lysis with polymer structure. Soft Matter, 2012, 8, 6744.	1.2	61
13	Selective Removal of Technetium from Water Using Graphene Oxide Membranes. Environmental Science & Technology, 2016, 50, 3875-3881.	4.6	53
14	A Coarse-Grained Model for Polyphenylene Dendrimers:Â Switching and Backfolding of Planar Three-Fold Core Dendrimers. Macromolecules, 2007, 40, 7044-7055.	2.2	52
15	Hydrogen Bonding and Dynamic Crossover in Polyamide-66: A Molecular Dynamics Simulation Study. Macromolecules, 2008, 41, 7211-7218.	2.2	50
16	Insights into the Polyhexamethylene Biguanide (PHMB) Mechanism of Action on Bacterial Membrane and DNA: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2020, 124, 4487-4497.	1.2	48
17	Charge Diffusion in Semiconducting Polymers: Analytical Relation between Polymer Rigidity and Time Scales for Intrachain and Interchain Hopping. Journal of Physical Chemistry Letters, 2014, 5, 2637-2641.	2.1	47
18	Fine-graining without coarse-graining: an easy and fast way to equilibrate dense polymer melts. Faraday Discussions, 2010, 144, 25-42.	1.6	45

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19	Propeneâ^'Norbornene Copolymers:Â Synthesis and Analysis of Polymer Structure by13C NMR Spectroscopy and ab Initio Chemical Shift Computations. Macromolecules, 2003, 36, 882-890.	2.2	44
20	Oxidative cyclodehydrogenation reaction for the design of extended 2D and 3D carbon nanostructures: A theoretical study. Chemical Physics, 2005, 314, 85-99.	0.9	44
21	Viscosity and Structural Alteration of a Coarse-Grained Model of Polystyrene under Steady Shear Flow Studied by Reverse Nonequilibrium Molecular Dynamics. Macromolecules, 2007, 40, 8087-8095.	2.2	37
22	Fast dynamics in coarse-grained polymer models: The effect of the hydrogen bonds. Journal of Chemical Physics, 2008, 129, 154904.	1.2	37
23	Constructing the phase diagram of sodium laurylethoxysulfate using dissipative particle dynamics. Journal of Colloid and Interface Science, 2019, 557, 34-44.	5.0	36
24	Coarseâ€grained methods for polymeric materials: enthalpyâ€•and entropyâ€driven models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 62-70.	6.2	34
25	Backmapping coarse-grained polymer models under sheared nonequilibrium conditions. Physical Chemistry Chemical Physics, 2009, 11, 1977.	1.3	32
26	In Silico Design and Characterization of Graphene Oxide Membranes with Variable Water Content and Flake Oxygen Content. ACS Nano, 2019, 13, 2995-3004.	7.3	32
27	Effect of Strain on the Photoisomerization and Stability of a Congested Azobenzenophane:Â A Combined Experimental and Computational Study. Journal of Physical Chemistry A, 2006, 110, 12385-12394.	1.1	30
28	Motor vehicle accidents and adolescents: An empirical study on their emotional and behavioral profiles, defense strategies and parental support. Transportation Research Part F: Traffic Psychology and Behaviour, 2015, 35, 28-36.	1.8	30
29	Mixing atoms and coarse-grained beads in modelling polymer melts. Journal of Chemical Physics, 2012, 137, 164111.	1.2	29
30	Relationship between the Affinity of PEO-PPO-PEO Block Copolymers for Biological Membranes and Their Cellular Effects. Pharmaceutical Research, 2012, 29, 1908-1918.	1.7	28
31	Reversible structural transition in nanoconfined ice. Physical Review B, 2017, 95, .	1.1	28
32	Computational characterisation of dried and hydrated graphene oxide membranes. Nanoscale, 2018, 10, 1946-1956.	2.8	28
33	Thermodynamics of the self-assembly of non-ionic chromonic molecules using atomistic simulations. The case of TP6EO2M in aqueous solution. Soft Matter, 2015, 11, 680-691.	1.2	27
34	Ab Initio Molecular Modeling of13C NMR Chemical Shifts of Polymers. 2. Propeneâ^'Norbornene Copolymersâ€. Macromolecules, 2003, 36, 891-899.	2.2	26
35	Solvent Structuring and Its Effect on the Polymer Structure and Processability: The Case of Waterâ€“Acetone Poly-Îµ-caprolactone Mixtures. Journal of Physical Chemistry B, 2014, 118, 13258-13267.	1.2	26
36	Dissipative particle dynamics simulations of tri-block co-polymer and water: Phase diagram validation and microstructure identification. Journal of Chemical Physics, 2018, 149, 184903.	1.2	26

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37	Why different water models predict different structures under 2D confinement. Journal of Computational Chemistry, 2018, 39, 2051-2059.	1.5	25
38	An experimental rheological phase diagram of a tri-block co-polymer in water validated against dissipative particle dynamics simulations. Soft Matter, 2019, 15, 1396-1404.	1.2	25
39	A classical force field for tetrahedral oxyanions developed using hydration properties: The examples of pertechnetate (TcO4â^') and sulfate (SO42â^'). Journal of Chemical Physics, 2015, 143, 174502.	1.2	24
40	Shape Persistence and Bistability of Planar Three-Fold Core Polyphenylene Dendrimers:Â A Molecular Dynamics Study. Journal of Physical Chemistry A, 2006, 110, 2214-2224.	1.1	23
41	Effect of Chain Length on the Partition Properties of Poly(ethylene oxide): Comparison between MARTINI Coarse-Grained and Atomistic Models. Journal of Physical Chemistry B, 2017, 121, 1601-1609.	1.2	22
42	A novel multiscale model for the simulation of polymer flash nano-precipitation. Chemical Engineering Science, 2017, 171, 485-494.	1.9	21
43	Semantic Interoperability and Characterization of Data Provenance in Computational Molecular Engineering. Journal of Chemical & Engineering Data, 2020, 65, 1313-1329.	1.0	21
44	Design Rules for Graphene and Carbon Nanotube Solvents and Dispersants. ACS Nano, 2018, 12, 1043-1049.	7.3	20
45	A QM/MD Coupling Method to Model the Ion-Induced Polarization of Graphene. Journal of Chemical Theory and Computation, 2020, 16, 5253-5263.	2.3	20
46	Role of Long-Range Electrostatic Interactions and Local Topology of the Hydrogen Bond Network in the Wettability of Fully and Partially Wetted Single and Multilayer Graphene. Journal of Physical Chemistry C, 2021, 125, 6367-6377.	1.5	20
47	How stable are amphiphilic dendrimers at the liquidâ€"liquid interface?. Soft Matter, 2013, 9, 6841-6850.	1.2	19
48	Identification of nucleation rate parameters with MD and validation of the CFD model for polymer particle precipitation. Chemical Engineering Research and Design, 2013, 91, 2275-2290.	2.7	19
49	The Relationship between Wormlike Micelle Scission Free Energy and Micellar Composition: The Case of Sodium Lauryl Ether Sulfate and Cocamidopropyl Betaine. Langmuir, 2020, 36, 12288-12298.	1.6	16
50	Thermodynamics of linear and star polymers at fluid interfaces. Soft Matter, 2015, 11, 81-93.	1.2	15
51	Prediction of Bulk Density and Molecular Packing in Model Dendrimers with Different Chain Stiffness. Macromolecules, 2010, 43, 9191-9197.	2.2	14
52	Stability of Amphiphilic Dendrimers at the Water/Air Interface. Journal of Physical Chemistry B, 2011, 115, 12019-12027.	1.2	14
53	A multiple time step scheme for multiresolved models of Macromolecules. Journal of Computational Chemistry, 2014, 35, 1199-1207.	1.5	14
54	Scalability of Coarseâ€Grained Potentials Generated from Iterative Boltzmann Inversion for Polymers: Case Study on Polycarbonates. Macromolecular Theory and Simulations, 2016, 25, 274-286.	0.6	14

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55	Unexpected Like-Charge Self-Assembly of a Biguanide-Based Antimicrobial Polyelectrolyte. Journal of Physical Chemistry Letters, 2016, 7, 3730-3735.	2.1	14
56	How the Incorporation of Pluronic Block Copolymers Modulates the Response of Lipid Membranes to Mechanical Stress. Langmuir, 2017, 33, 13284-13294.	1.6	14
57	Polyisoprene local dynamics in solution: Comparison between molecular dynamics simulations and high order diffusion theory. Journal of Chemical Physics, 2001, 114, 1876-1886.	1.2	13
58	Molecular dynamics simulations of polyaminoamide (PAMAM) dendrimer aggregates: molecular shape, hydrogen bonds and local dynamics. Soft Matter, 2009, , .	1.2	13
59	Calculation of the work of adhesion of polyisoprene on graphite by molecular dynamics simulations. Soft Materials, 2020, 18, 140-149.	0.8	13
60	A molecular simulation study into the stability of hydrated graphene nanochannels used in nanofluidics devices. Nanoscale, 2022, 14, 3467-3479.	2.8	13
61	Wettability of graphite under 2D confinement. Carbon, 2022, 198, 132-141.	5.4	13
62	Propene-Norbornene Copolymers: Synthesis and Microstructure. Macromolecular Symposia, 2001, 169, 39-50.	0.4	12
63	High-throughput molecular simulations reveal the origin of ion free energy barriers in graphene oxide membranes. Nanoscale, 2021, 13, 13693-13702.	2.8	12
64	Dynamically Polarizable Force Fields for Surface Simulations via Multi-output Classification Neural Networks. Journal of Chemical Theory and Computation, 2021, 17, 4477-4485.	2.3	11
65	Ab initio molecular modeling of13C NMR chemical shifts of polymers. 1. Ethylene-norbornene copolymers. International Journal of Quantum Chemistry, 2002, 88, 663-669.	1.0	10
66	Glass Transition Temperature and Chain Flexibility of Ethylene-Norbornene Copolymers from Molecular Dynamics Simulations. Macromolecular Theory and Simulations, 2006, 15, 457-468.	0.6	10
67	Local and global dynamics of multi-resolved polymer chains: Effects of the interactions atoms-beads on the dynamic of the chains. Journal of Chemical Physics, 2017, 146, 084905.	1.2	10
68	Extended Charge-On-Particle Optimized Potentials for Liquid Simulation Acetone Model: The Case of Acetoneâ€“Water Mixtures. Journal of Physical Chemistry B, 2018, 122, 5234-5241.	1.2	10
69	Comparison of equilibrium techniques for the viscosity calculation from DPD simulations. Soft Matter, 2021, 17, 8343-8353.	1.2	10
70	Scaling Behavior of Polymers at Liquid/Liquid Interfaces. ACS Macro Letters, 2015, 4, 1089-1093.	2.3	9
71	A Theoretical and Empirical Linkage between Road Accidents and Binge Eating Behaviors in Adolescence. International Journal of Environmental Research and Public Health, 2018, 15, 355.	1.2	8
72	Effects of Graphite and Plasticizers on the Structure of Highly Entangled Polyisoprene Melts. ACS Applied Polymer Materials, 2020, 2, 317-325.	2.0	8

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73	Amphiphilic copolymers change the nature of the ordered-to-disordered phase transition of lipid membranes from discontinuous to continuous. Physical Chemistry Chemical Physics, 2019, 21, 13746-13757.	1.3	6
74	Cross-over in the dynamics of polymer confined between two liquids of different viscosity. Interface Focus, 2019, 9, 20180074.	1.5	6
75	A different approach to dual-scale models. Journal of Computational Physics, 2020, 413, 109465.	1.9	6
76	Dealloying layered PdBi₂ nanoflakes to palladium hydride leads to enhanced electrocatalytic N₂ reduction. Journal of Materials Chemistry A, 2022, 10, 11904-11916.	5.2	6
77	The role of surface ionisation in the hydration-induced swelling of graphene oxide membranes. Journal of Membrane Science, 2022, 653, 120489.	4.1	6
78	<scp>MARTINI</scp> coarseâ€grained model for polyâ€îµâ€caprolactone in acetoneâ€water mixtures. Canadian Journal of Chemical Engineering, 2020, 98, 1868-1879.	0.9	5
79	Mechanical hydrolysis imparts self-destruction of water molecules under steric confinement. Physical Chemistry Chemical Physics, 2021, 23, 5999-6008.	1.3	5
80	Multiscale modelling of heterogeneous fillers in polymer composites: the case of polyisoprene and carbon black. Journal of Physics Condensed Matter, 2021, 33, 194003.	0.7	5
81	Reply to: Random interstratification in hydrated graphene oxide membranes and implications for seawater desalination. Nature Nanotechnology, 2022, 17, 134-135.	15.6	5
82	Adsorption of amphiphilic grafted polymers as polymer corrosion inhibitors: insights from mesoscopic simulations. Physical Chemistry Chemical Physics, 2022, 24, 11992-12001.	1.3	5
83	Motor Vehicle Collisions during Adolescence: The Role of Alexithymic Traits and Defense Strategies. Behavioral Sciences (Basel, Switzerland), 2021, 11, 79.	1.0	4
84	Development of hybrid coarse-grained atomistic models for rapid assessment of local structuring of polymeric semiconductors. Molecular Systems Design and Engineering, 2022, 7, 294-305.	1.7	3
85	Diversification of services: the technological window in Liguria. World Patent Information, 2002, 24, 233-236.	0.7	2
86	Simulation of macromolecule self-assembly in solution: A multiscale approach. AIP Conference Proceedings, 2015, , .	0.3	2
87	New customers for PatLib Genoa â€“ Good practice for attracting more clients. World Patent Information, 2007, 29, 246-249.	0.7	0
88	Distance learning training in genetics and genomics practices for Italian physicians. European Journal of Public Health, 2017, 27, .	0.1	0
89	Coarse-Grained and Hybrid Simulations of Nanostructures. , 2015, , 1-10.		0
90	Coarse-Grained and Hybrid Simulations of Nanostructures. , 2016, , 597-604.		0