

# Paola Carbone

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

82  
papers

4,538  
citations

24  
h-index

67  
g-index

93  
ext. papers

5,284  
ext. citations

5.6  
avg, IF

5.67  
L-index

#	Paper	IF	Citations
82	Precise and ultrafast molecular sieving through graphene oxide membranes. <i>Science</i> , <b>2014</b> , 343, 752-4	33.3	1664
81	Tunable sieving of ions using graphene oxide membranes. <i>Nature Nanotechnology</i> , <b>2017</b> , 12, 546-550	28.7	960
80	Temperature-Transferable Coarse-Grained Potentials for Ethylbenzene, Polystyrene, and Their Mixtures. <i>Macromolecules</i> , <b>2008</b> , 41, 9919-9929	5.5	174
79	Transferability of coarse-grained force fields: the polymer case. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 064904	3.9	171
78	Van der Waals pressure and its effect on trapped interlayer molecules. <i>Nature Communications</i> , <b>2016</b> , 7, 12168	17.4	91
77	How good are coarse-grained polymer models? A comparison for atactic polystyrene. <i>ChemPhysChem</i> , <b>2012</b> , 13, 3428-39	3.2	85
76	Interactions of PEO-PPO-PEO block copolymers with lipid membranes: a computational and experimental study linking membrane lysis with polymer structure. <i>Soft Matter</i> , <b>2012</b> , 8, 6744	3.6	54
75	Studying long-time dynamics of imidazolium-based ionic liquids with a systematically coarse-grained model. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 4714-24	3.6	54
74	Coarse-graining poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) (PEO-PPO-PEO) block copolymers using the MARTINI force field. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 1648-59	3.4	52
73	A Coarse-Grained Model for Polyphenylene Dendrimers: Switching and Backfolding of Planar Three-Fold Core Dendrimers. <i>Macromolecules</i> , <b>2007</b> , 40, 7044-7055	5.5	51
72	Effective Polarization in Pairwise Potentials at the Graphene-Electrolyte Interface. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 703-708	6.4	43
71	Hydrogen Bonding and Dynamic Crossover in Polyamide-66: A Molecular Dynamics Simulation Study. <i>Macromolecules</i> , <b>2008</b> , 41, 7211-7218	5.5	42
70	Oxidative cyclodehydrogenation reaction for the design of extended 2D and 3D carbon nanostructures: A theoretical study. <i>Chemical Physics</i> , <b>2005</b> , 314, 85-99	2.3	42
69	Selective Removal of Technetium from Water Using Graphene Oxide Membranes. <i>Environmental Science &amp; Technology</i> , <b>2016</b> , 50, 3875-81	10.3	41
68	Charge Diffusion in Semiconducting Polymers: Analytical Relation between Polymer Rigidity and Time Scales for Intrachain and Interchain Hopping. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 2637-41	6.4	40
67	Fine-graining without coarse-graining: an easy and fast way to equilibrate dense polymer melts. <i>Faraday Discussions</i> , <b>2010</b> , 144, 25-42; discussion 93-110, 467-81	3.6	40
66	A multiscale approach to model hydrogen bonding: The case of polyamide. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 224907	3.9	37

65	PropeneNorbornene Copolymers: Synthesis and Analysis of Polymer Structure by $^{13}\text{C}$ NMR Spectroscopy and ab Initio Chemical Shift Computations. <i>Macromolecules</i> , <b>2003</b> , 36, 882-890	5.5	36
64	Viscosity and Structural Alteration of a Coarse-Grained Model of Polystyrene under Steady Shear Flow Studied by Reverse Nonequilibrium Molecular Dynamics. <i>Macromolecules</i> , <b>2007</b> , 40, 8087-8095	5.5	32
63	Fast dynamics in coarse-grained polymer models: the effect of the hydrogen bonds. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 154904	3.9	31
62	Backmapping coarse-grained polymer models under sheared nonequilibrium conditions. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 1977-88	3.6	30
61	Coarse-grained methods for polymeric materials: enthalpy- and entropy-driven models. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2014</b> , 4, 62-70	7.9	28
60	Effect of strain on the photoisomerization and stability of a congested azobenzenophane: a combined experimental and computational study. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 12385-94	2.8	28
59	Thermodynamics of the self-assembly of non-ionic chromonic molecules using atomistic simulations. The case of TP6EO2M in aqueous solution. <i>Soft Matter</i> , <b>2015</b> , 11, 680-91	3.6	24
58	Ab Initio Molecular Modeling of $^{13}\text{C}$ NMR Chemical Shifts of Polymers. 2. PropeneNorbornene Copolymers <i>Macromolecules</i> , <b>2003</b> , 36, 891-899	5.5	24
57	Constructing the phase diagram of sodium laurylthoxysulfate using dissipative particle dynamics. <i>Journal of Colloid and Interface Science</i> , <b>2019</b> , 557, 34-44	9.3	23
56	Motor vehicle accidents and adolescents: An empirical study on their emotional and behavioral profiles, defense strategies and parental support. <i>Transportation Research Part F: Traffic Psychology and Behaviour</i> , <b>2015</b> , 35, 28-36	4.5	23
55	Mixing atoms and coarse-grained beads in modelling polymer melts. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 164111	3.9	23
54	In Silico Design and Characterization of Graphene Oxide Membranes with Variable Water Content and Flake Oxygen Content. <i>ACS Nano</i> , <b>2019</b> , 13, 2995-3004	16.7	22
53	Shape persistence and bistability of planar three-fold core polyphenylene dendrimers: a molecular dynamics study. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 2214-24	2.8	22
52	Reversible structural transition in nanoconfined ice. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	21
51	Insights into the Polyhexamethylene Biguanide (PHMB) Mechanism of Action on Bacterial Membrane and DNA: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 4487-4497 <sup>3-4</sup>	3.4	21
50	Solvent structuring and its effect on the polymer structure and processability: the case of water-acetone poly- $\epsilon$ -caprolactone mixtures. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 13258-67	3.4	21
49	Relationship between the affinity of PEO-PPO-PEO block copolymers for biological membranes and their cellular effects. <i>Pharmaceutical Research</i> , <b>2012</b> , 29, 1908-18	4.5	21
48	Computational characterisation of dried and hydrated graphene oxide membranes. <i>Nanoscale</i> , <b>2018</b> , 10, 1946-1956	7.7	20

47	Dissipative particle dynamics simulations of tri-block co-polymer and water: Phase diagram validation and microstructure identification. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 184903	3.9	19
46	Effect of Chain Length on the Partition Properties of Poly(ethylene oxide): Comparison between MARTINI Coarse-Grained and Atomistic Models. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 1601-1609	3.4	18
45	How stable are amphiphilic dendrimers at the liquid-liquid interface?. <i>Soft Matter</i> , <b>2013</b> , 9, 6841-6850	3.6	18
44	A classical force field for tetrahedral oxyanions developed using hydration properties: The examples of pertechnetate (TcO <sub>4</sub> <sup>-</sup> ) and sulfate (SO <sub>4</sub> <sup>2-</sup> ). <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 174502	3.9	17
43	Identification of nucleation rate parameters with MD and validation of the CFD model for polymer particle precipitation. <i>Chemical Engineering Research and Design</i> , <b>2013</b> , 91, 2275-2290	5.5	17
42	Why different water models predict different structures under 2D confinement. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 2051-2059	3.5	17
41	A novel multiscale model for the simulation of polymer flash nano-precipitation. <i>Chemical Engineering Science</i> , <b>2017</b> , 171, 485-494	4.4	16
40	Semantic Interoperability and Characterization of Data Provenance in Computational Molecular Engineering. <i>Journal of Chemical &amp; Engineering Data</i> , <b>2020</b> , 65, 1313-1329	2.8	16
39	An experimental rheological phase diagram of a tri-block co-polymer in water validated against dissipative particle dynamics simulations. <i>Soft Matter</i> , <b>2019</b> , 15, 1396-1404	3.6	14
38	Stability of amphiphilic dendrimers at the water/air interface. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 12019-27	3.4	14
37	A multiple time step scheme for multiresolved models of macromolecules. <i>Journal of Computational Chemistry</i> , <b>2014</b> , 35, 1199-207	3.5	13
36	Prediction of Bulk Density and Molecular Packing in Model Dendrimers with Different Chain Stiffness. <i>Macromolecules</i> , <b>2010</b> , 43, 9191-9197	5.5	13
35	Thermodynamics of linear and star polymers at fluid interfaces. <i>Soft Matter</i> , <b>2015</b> , 11, 81-93	3.6	12
34	Design Rules for Graphene and Carbon Nanotube Solvents and Dispersants. <i>ACS Nano</i> , <b>2018</b> , 12, 1043-1049	4.7	12
33	Molecular dynamics simulations of polyaminoamide (PAMAM) dendrimer aggregates: molecular shape, hydrogen bonds and local dynamics. <i>Soft Matter</i> , <b>2009</b> ,	3.6	12
32	Polyisoprene local dynamics in solution: Comparison between molecular dynamics simulations and high order diffusion theory. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 1876-1886	3.9	12
31	How the Incorporation of Pluronic Block Copolymers Modulates the Response of Lipid Membranes to Mechanical Stress. <i>Langmuir</i> , <b>2017</b> , 33, 13284-13294	4	11
30	Scalability of Coarse-Grained Potentials Generated from Iterative Boltzmann Inversion for Polymers: Case Study on Polycarbonates. <i>Macromolecular Theory and Simulations</i> , <b>2016</b> , 25, 274-286	1.5	11

29	Ab initio molecular modeling of <sup>13</sup> C NMR chemical shifts of polymers. 1. Ethylene-Norbornene copolymers. <i>International Journal of Quantum Chemistry</i> , <b>2002</b> , 88, 663-669	2.1	10
28	Glass Transition Temperature and Chain Flexibility of Ethylene-Norbornene Copolymers from Molecular Dynamics Simulations. <i>Macromolecular Theory and Simulations</i> , <b>2006</b> , 15, 457-468	1.5	9
27	Unexpected Like-Charge Self-Assembly of a Biguanide-Based Antimicrobial Polyelectrolyte. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 3730-3735	6.4	9
26	A QM/MD Coupling Method to Model the Ion-Induced Polarization of Graphene. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 5253-5263	6.4	8
25	Extended Charge-On-Particle Optimized Potentials for Liquid Simulation Acetone Model: The Case of Acetone-Water Mixtures. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 5234-5241	3.4	8
24	Effects of Graphite and Plasticizers on the Structure of Highly Entangled Polyisoprene Melts. <i>ACS Applied Polymer Materials</i> , <b>2020</b> , 2, 317-325	4.3	8
23	The Relationship between Wormlike Micelle Scission Free Energy and Micellar Composition: The Case of Sodium Lauryl Ether Sulfate and Cocamidopropyl Betaine. <i>Langmuir</i> , <b>2020</b> , 36, 12288-12298	4	8
22	Local and global dynamics of multi-resolved polymer chains: Effects of the interactions atoms-beads on the dynamic of the chains. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 084905	3.9	7
21	A Theoretical and Empirical Linkage between Road Accidents and Binge Eating Behaviors in Adolescence. <i>International Journal of Environmental Research and Public Health</i> , <b>2018</b> , 15,	4.6	7
20	Scaling Behavior of Polymers at Liquid/Liquid Interfaces. <i>ACS Macro Letters</i> , <b>2015</b> , 4, 1089-1093	6.6	6
19	Calculation of the work of adhesion of polyisoprene on graphite by molecular dynamics simulations. <i>Soft Materials</i> , <b>2020</b> , 18, 140-149	1.7	6
18	Propene-Norbornene Copolymers: Synthesis and Microstructure. <i>Macromolecular Symposia</i> , <b>2001</b> , 169, 39-50	0.8	5
17	MARTINI coarse-grained model for poly-ε-caprolactone in acetone-water mixtures. <i>Canadian Journal of Chemical Engineering</i> , <b>2020</b> , 98, 1868-1879	2.3	4
16	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. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 6367-6377	3.8	4
15	A different approach to dual-scale models. <i>Journal of Computational Physics</i> , <b>2020</b> , 413, 109465	4.1	3
14	Amphiphilic copolymers change the nature of the ordered-to-disordered phase transition of lipid membranes from discontinuous to continuous. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 13746-13757	3.6	2
13	Cross-over in the dynamics of polymer confined between two liquids of different viscosity. <i>Interface Focus</i> , <b>2019</b> , 9, 20180074	3.9	2
12	Diversification of services: the technological window in Liguria. <i>World Patent Information</i> , <b>2002</b> , 24, 233-236		2

11	Reply to: Random interstratification in hydrated graphene oxide membranes and implications for seawater desalination.. <i>Nature Nanotechnology</i> , <b>2022</b> ,	28.7	2
10	Multiscale modelling of heterogeneous fillers in polymer composites: the case of polyisoprene and carbon black. <i>Journal of Physics Condensed Matter</i> , <b>2021</b> , 33,	1.8	2
9	Motor Vehicle Collisions during Adolescence: The Role of Alexithymic Traits and Defense Strategies. <i>Behavioral Sciences (Basel, Switzerland)</i> , <b>2021</b> , 11,	2.3	2
8	Mechanical hydrolysis imparts self-destruction of water molecules under steric confinement. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 5999-6008	3.6	2
7	Comparison of equilibrium techniques for the viscosity calculation from DPD simulations. <i>Soft Matter</i> , <b>2021</b> , 17, 8343-8353	3.6	2
6	High-throughput molecular simulations reveal the origin of ion free energy barriers in graphene oxide membranes. <i>Nanoscale</i> , <b>2021</b> , 13, 13693-13702	7.7	2
5	Dynamically Polarizable Force Fields for Surface Simulations via Multi-output Classification Neural Networks. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 4477-4485	6.4	2
4	Simulation of macromolecule self-assembly in solution: A multiscale approach <b>2015</b> ,		1
3	Adsorption of amphiphilic grafted polymers as polymer corrosion inhibitors: insights from mesoscopic simulations.. <i>Physical Chemistry Chemical Physics</i> , <b>2022</b> , 24, 11992-12001	3.6	0
2	New customers for PatLib Genoa [Good practice for attracting more clients. <i>World Patent Information</i> , <b>2007</b> , 29, 246-249	1.4	
1	The role of surface ionisation in the hydration-induced swelling of graphene oxide membranes. <i>Journal of Membrane Science</i> , <b>2022</b> , 653, 120489	9.6	