Paola Carbone

List of Publications by Year in Descending Order

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	Reply to: Random interstratification in hydrated graphene oxide membranes and implications for seawater desalination.. *Nature Nanotechnology*, **2022**,	28.7	2
81	The role of surface ionisation in the hydration-induced swelling of graphene oxide membranes. *Journal of Membrane Science*, **2022**, 653, 120489	9.6	
80	Adsorption of amphiphilic grafted polymers as polymer corrosion inhibitors: insights from mesoscopic simulations.. *Physical Chemistry Chemical Physics*, **2022**, 24, 11992-12001	3.6	0
79	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	3.8	4
78	Multiscale modelling of heterogeneous fillers in polymer composites: the case of polyisoprene and carbon black. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	2
77	Motor Vehicle Collisions during Adolescence: The Role of Alexithymic Traits and Defense Strategies. *Behavioral Sciences (Basel, Switzerland)*, **2021**, 11,	2.3	2
76	Mechanical hydrolysis imparts self-destruction of water molecules under steric confinement. *Physical Chemistry Chemical Physics*, **2021**, 23, 5999-6008	3.6	2
75	Comparison of equilibrium techniques for the viscosity calculation from DPD simulations. *Soft Matter*, **2021**, 17, 8343-8353	3.6	2
74	High-throughput molecular simulations reveal the origin of ion free energy barriers in graphene oxide membranes. *Nanoscale*, **2021**, 13, 13693-13702	7.7	2
73	Dynamically Polarizable Force Fields for Surface Simulations via Multi-output Classification Neural Networks. *Journal of Chemical Theory and Computation*, **2021**, 17, 4477-4485	6.4	2
72	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	3.4	21
71	A QM/MD Coupling Method to Model the Ion-Induced Polarization of Graphene. *Journal of Chemical Theory and Computation*, **2020**, 16, 5253-5263	6.4	8
70	MARTINI coarse-grained model for poly-□caprolactone in acetone-water mixtures. *Canadian Journal of Chemical Engineering*, **2020**, 98, 1868-1879	2.3	4
69	Semantic Interoperability and Characterization of Data Provenance in Computational Molecular Engineering. *Journal of Chemical & Engineering Data*, **2020**, 65, 1313-1329	2.8	16
68	Effects of Graphite and Plasticizers on the Structure of Highly Entangled Polyisoprene Melts. *ACS Applied Polymer Materials*, **2020**, 2, 317-325	4.3	8
67	Calculation of the work of adhesion of polyisoprene on graphite by molecular dynamics simulations. *Soft Materials*, **2020**, 18, 140-149	1.7	6
66	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	4	8

65	A different approach to dual-scale models. *Journal of Computational Physics*, **2020**, 413, 109465	4.1	3
64	Constructing the phase diagram of sodium laurylethoxysulfate using dissipative particle dynamics. *Journal of Colloid and Interface Science*, **2019**, 557, 34-44	9.3	23
63	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	3.6	14
62	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	3.6	2
61	Cross-over in the dynamics of polymer confined between two liquids of different viscosity. *Interface Focus*, **2019**, 9, 20180074	3.9	2
60	In Silico Design and Characterization of Graphene Oxide Membranes with Variable Water Content and Flake Oxygen Content. *ACS Nano*, **2019**, 13, 2995-3004	16.7	22
59	Design Rules for Graphene and Carbon Nanotube Solvents and Dispersants. *ACS Nano*, **2018**, 12, 1043-1049	14.7	12
58	Computational characterisation of dried and hydrated graphene oxide membranes. *Nanoscale*, **2018**, 10, 1946-1956	7.7	20
57	Extended Charge-On-Particle Optimized Potentials for Liquid Simulation Acetone Model: The Case of Acetone-Water Mixtures. *Journal of Physical Chemistry B*, **2018**, 122, 5234-5241	3.4	8
56	A Theoretical and Empirical Linkage between Road Accidents and Binge Eating Behaviors in Adolescence. *International Journal of Environmental Research and Public Health*, **2018**, 15,	4.6	7
55	Dissipative particle dynamics simulations of tri-block co-polymer and water: Phase diagram validation and microstructure identification. *Journal of Chemical Physics*, **2018**, 149, 184903	3.9	19
54	Why different water models predict different structures under 2D confinement. *Journal of Computational Chemistry*, **2018**, 39, 2051-2059	3.5	17
53	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	3.4	18
52	Effective Polarization in Pairwise Potentials at the Graphene-Electrolyte Interface. *Journal of Physical Chemistry Letters*, **2017**, 8, 703-708	6.4	43
51	Reversible structural transition in nanoconfined ice. *Physical Review B*, **2017**, 95,	3.3	21
50	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	3.9	7
49	Tunable sieving of ions using graphene oxide membranes. *Nature Nanotechnology*, **2017**, 12, 546-550	28.7	960
48	How the Incorporation of Pluronic Block Copolymers Modulates the Response of Lipid Membranes to Mechanical Stress. *Langmuir*, **2017**, 33, 13284-13294	4	11

47	A novel multiscale model for the simulation of polymer flash nano-precipitation. *Chemical Engineering Science*, **2017**, 171, 485-494	4.4	16
46	Van der Waals pressure and its effect on trapped interlayer molecules. *Nature Communications*, **2016**, 7, 12168	17.4	91
45	Selective Removal of Technetium from Water Using Graphene Oxide Membranes. *Environmental Science & Technology*, **2016**, 50, 3875-81	10.3	41
44	Scalability of Coarse-Grained Potentials Generated from Iterative Boltzmann Inversion for Polymers: Case Study on Polycarbonates. *Macromolecular Theory and Simulations*, **2016**, 25, 274-286	1.5	11
43	Unexpected Like-Charge Self-Assembly of a Biguanide-Based Antimicrobial Polyelectrolyte. *Journal of Physical Chemistry Letters*, **2016**, 7, 3730-3735	6.4	9
42	A multiscale approach to model hydrogen bonding: The case of polyamide. *Journal of Chemical Physics*, **2015**, 142, 224907	3.9	37
41	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	4.5	23
40	Scaling Behavior of Polymers at Liquid/Liquid Interfaces. *ACS Macro Letters*, **2015**, 4, 1089-1093	6.6	6
39	Thermodynamics of the self-assembly of non-ionic chromonic molecules using atomistic simulations. The case of TP6EO2M in aqueous solution. *Soft Matter*, **2015**, 11, 680-91	3.6	24
38	Thermodynamics of linear and star polymers at fluid interfaces. *Soft Matter*, **2015**, 11, 81-93	3.6	12
37	Simulation of macromolecule self-assembly in solution: A multiscale approach **2015**,		1
36	A classical force field for tetrahedral oxyanions developed using hydration properties: The examples of pertechnetate (TcO4(-)) and sulfate (SO4(2-)). *Journal of Chemical Physics*, **2015**, 143, 174502	3.9	17
35	Precise and ultrafast molecular sieving through graphene oxide membranes. *Science*, **2014**, 343, 752-4	33.3	1664
34	A multiple time step scheme for multiresolved models of macromolecules. *Journal of Computational Chemistry*, **2014**, 35, 1199-207	3.5	13
33	Solvent structuring and its effect on the polymer structure and processability: the case of water-acetone poly-Ɛ-caprolactone mixtures. *Journal of Physical Chemistry B*, **2014**, 118, 13258-67	3.4	21
32	Coarse-graining poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) (PEO-PPO-PEO) block copolymers using the MARTINI force field. *Journal of Physical Chemistry B*, **2014**, 118, 1648-59	3.4	52
31	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, 2637-41	6.4	40
30	Coarse-grained methods for polymeric materials: enthalpy- and entropy-driven models. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 62-70	7.9	28

29	How stable are amphiphilic dendrimers at the liquid–liquid interface?. *Soft Matter*, **2013**, 9, 6841-6850	3.6	18
28	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	5.5	17
27	Interactions of PEO–PPO–PEO block copolymers with lipid membranes: a computational and experimental study linking membrane lysis with polymer structure. *Soft Matter*, **2012**, 8, 6744	3.6	54
26	How good are coarse-grained polymer models? A comparison for atactic polystyrene. *ChemPhysChem*, **2012**, 13, 3428-39	3.2	85
25	Relationship between the affinity of PEO-PPO-PEO block copolymers for biological membranes and their cellular effects. *Pharmaceutical Research*, **2012**, 29, 1908-18	4.5	21
24	Mixing atoms and coarse-grained beads in modelling polymer melts. *Journal of Chemical Physics*, **2012**, 137, 164111	3.9	23
23	Stability of amphiphilic dendrimers at the water/air interface. *Journal of Physical Chemistry B*, **2011**, 115, 12019-27	3.4	14
22	Fine-graining without coarse-graining: an easy and fast way to equilibrate dense polymer melts. *Faraday Discussions*, **2010**, 144, 25-42; discussion 93-110, 467-81	3.6	40
21	Prediction of Bulk Density and Molecular Packing in Model Dendrimers with Different Chain Stiffness. *Macromolecules*, **2010**, 43, 9191-9197	5.5	13
20	Studying long-time dynamics of imidazolium-based ionic liquids with a systematically coarse-grained model. *Physical Chemistry Chemical Physics*, **2010**, 12, 4714-24	3.6	54
19	Molecular dynamics simulations of polyaminoamide (PAMAM) dendrimer aggregates: molecular shape, hydrogen bonds and local dynamics. *Soft Matter*, **2009**,	3.6	12
18	Backmapping coarse-grained polymer models under sheared nonequilibrium conditions. *Physical Chemistry Chemical Physics*, **2009**, 11, 1977-88	3.6	30
17	Transferability of coarse-grained force fields: the polymer case. *Journal of Chemical Physics*, **2008**, 128, 064904	3.9	171
16	Temperature-Transferable Coarse-Grained Potentials for Ethylbenzene, Polystyrene, and Their Mixtures. *Macromolecules*, **2008**, 41, 9919-9929	5.5	174
15	Hydrogen Bonding and Dynamic Crossover in Polyamide-66: A Molecular Dynamics Simulation Study. *Macromolecules*, **2008**, 41, 7211-7218	5.5	42
14	Fast dynamics in coarse-grained polymer models: the effect of the hydrogen bonds. *Journal of Chemical Physics*, **2008**, 129, 154904	3.9	31
13	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	5.5	32
12	A Coarse-Grained Model for Polyphenylene Dendrimers: Switching and Backfolding of Planar Three-Fold Core Dendrimers. *Macromolecules*, **2007**, 40, 7044-7055	5.5	51

11	New customers for PatLib Genoa Good practice for attracting more clients. *World Patent Information*, **2007**, 29, 246-249	1.4	
10	Glass Transition Temperature and Chain Flexibility of Ethylene-Norbornene Copolymers from Molecular Dynamics Simulations. *Macromolecular Theory and Simulations*, **2006**, 15, 457-468	1.5	9
9	Effect of strain on the photoisomerization and stability of a congested azobenzenophane: a combined experimental and computational study. *Journal of Physical Chemistry A*, **2006**, 110, 12385-94	2.8	28
8	Shape persistence and bistability of planar three-fold core polyphenylene dendrimers: a molecular dynamics study. *Journal of Physical Chemistry A*, **2006**, 110, 2214-24	2.8	22
7	Oxidative cyclodehydrogenation reaction for the design of extended 2D and 3D carbon nanostructures: A theoretical study. *Chemical Physics*, **2005**, 314, 85-99	2.3	42
6	Ab Initio Molecular Modeling of 13C NMR Chemical Shifts of Polymers. 2. Propene Norbornene Copolymers *Macromolecules*, **2003**, 36, 891-899	5.5	24
5	Propene Norbornene Copolymers: Synthesis and Analysis of Polymer Structure by13C NMR Spectroscopy and ab Initio Chemical Shift Computations. *Macromolecules*, **2003**, 36, 882-890	5.5	36
4	Diversification of services: the technological window in Liguria. *World Patent Information*, **2002**, 24, 233-236	1	2
3	Ab initio molecular modeling of 13C NMR chemical shifts of polymers. 1. Ethylene norbornene copolymers. *International Journal of Quantum Chemistry*, **2002**, 88, 663-669	2.1	10
2	Propene-Norbornene Copolymers: Synthesis and Microstructure. *Macromolecular Symposia*, **2001**, 169, 39-50	0.8	5
1	Polyisoprene local dynamics in solution: Comparison between molecular dynamics simulations and high order diffusion theory. *Journal of Chemical Physics*, **2001**, 114, 1876-1886	3.9	12