Riccardo Alessandri

List of Publications by Year
in descending order

19 papers	1,762 citations	516215 16 h-index	794141 19 g-index
28 all docs	28 docs citations	28 times ranked	1729 citing authors

#	Article	IF	Citations
1	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
2	Enhancing Molecular nâ€Type Doping of Donorâ€“Acceptor Copolymers by Tailoring Side Chains. Advanced Materials, 2018, 30, 1704630.	11.1	217
3	Pitfalls of the Martini Model. Journal of Chemical Theory and Computation, 2019, 15, 5448-5460.	2.3	159
4	Proteinâ€“ligand binding with the coarse-grained Martini model. Nature Communications, 2020, 11, 3714.	5.8	139
5	Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. Journal of the American Chemical Society, 2017, 139, 3697-3705.	6.6	133
6	N-type organic thermoelectrics: demonstration of ZTâ€‰>â€‰0.3. Nature Communications, 2020, 11, 5694.	5.8	98
7	Enhancing doping efficiency by improving host-dopant miscibility for fullerene-based n-type thermoelectrics. Journal of Materials Chemistry A, 2017, 5, 21234-21241.	5.2	73
8	Martini 3 Coarseâ€Grained Force Field: Small Molecules. Advanced Theory and Simulations, 2022, 5, .	1.3	72
9	The Martini Model in Materials Science. Advanced Materials, 2021, 33, e2008635.	11.1	63
10	Two decades of Martini: Better beads, broader scope. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	58
11	Polyply; a python suite for facilitating simulations of macromolecules and nanomaterials. Nature Communications, 2022, 13, 68.	5.8	48
12	Resolving Donorâ€“Acceptor Interfaces and Charge Carrier Energy Levels of Organic Semiconductors with Polar Side Chains. Advanced Functional Materials, 2020, 30, 2004799.	7.8	28
13	Can the Dielectric Constant of Fullerene Derivatives Be Enhanced by Side-Chain Manipulation? A Predictive First-Principles Computational Study. Journal of Physical Chemistry A, 2018, 122, 3919-3926.	1.1	24
14	How Ethylene Glycol Chains Enhance the Dielectric Constant of Organic Semiconductors: Molecular Origin and Frequency Dependence. ACS Applied Materials & Interfaces, 2020, 12, 17783-17789.	4.0	23
15	Crystal Field in Rareâ€Earth Complexes: From Electrostatics to Bonding. Chemistry - A European Journal, 2018, 24, 5538-5550.	1.7	21
16	Multiscale modeling of molecular structure and optical properties of complex supramolecular aggregates. Chemical Science, 2020, 11, 11514-11524.	3.7	18
17	Molecular versus Excitonic Disorder in Individual Artificial Light-Harvesting Systems. Journal of the American Chemical Society, 2020, 142, 18073-18085.	6.6	13
18	Fullerene derivatives with oligoethyleneâ€“glycol side chains: an investigation on the origin of their outstanding transport properties. Journal of Materials Chemistry C, 2021, 9, 16217-16225.	2.7	10

#	Article	IF	Citations
19	Comparing Dimerization Free Energies and Binding Modes of Small Aromatic Molecules with Different Force Fields. Molecules, 2021, 26, 6069.	1.7	3