Carlos Avendano

List of Publications by Year
in descending order

36 papers	1,716 citations	394421 19 h-index	345221 36 g-index
37 all docs	37 docs citations	37 times ranked	1198 citing authors

#	Article	IF	Citations
1	Accurate statistical associating fluid theory for chain molecules formed from Mie segments. Journal of Chemical Physics, 2013, 139, 154504.	3.0	382
2	Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments. Journal of Chemical Physics, 2014, 140, 054107.	3.0	225
3	SAFT-Î³ Force Field for the Simulation of Molecular Fluids. 1. A Single-Site Coarse Grained Model of Carbon Dioxide. Journal of Physical Chemistry B, 2011, 115, 11154-11169.	2.6	200
4	SAFT-Î³ Force Field for the Simulation of Molecular Fluids: 2. Coarse-Grained Models of Greenhouse Gases, Refrigerants, and Long Alkanes. Journal of Physical Chemistry B, 2013, 117, 2717-2733.	2.6	126
5	Phase behavior of rounded hard-squares. Soft Matter, 2012, 8, 4675.	2.7	104
6	SAFT-Î³force field for the simulation of molecular fluids: 3. Coarse-grained models of benzene and hetero-group models ofn-decylbenzene. Molecular Physics, 2012, 110, 1189-1203.	1.7	82
7	SAFT-Î³ force field for the simulation of molecular fluids: 4. A single-site coarse-grained model of water applicable over a wide temperature range. Molecular Physics, 2015, 113, 1228-1249.	1.7	72
8	Transport diffusivities of fluids in nanopores by non-equilibrium molecular dynamics simulation. Molecular Simulation, 2012, 38, 540-553.	2.0	61
9	Monte Carlo simulations of primitive models for ionic systems using the Wolf method. Molecular Physics, 2006, 104, 1475-1486.	1.7	48
10	Assembly of porous smectic structures formed from interlocking high-symmetry planar nanorings. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9699-9703.	7.1	39
11	SAFT-Î³ Force Field for the Simulation of Molecular Fluids. 5. Hetero-Group Coarse-Grained Models of Linear Alkanes and the Importance of Intramolecular Interactions. Journal of Physical Chemistry B, 2018, 122, 9161-9177.	2.6	37
12	Packing, entropic patchiness, and self-assembly of non-convex colloidal particles: A simulation perspective. Current Opinion in Colloid and Interface Science, 2017, 30, 62-69.	7.4	36
13	Coarseâ€grained methods for polymeric materials: enthalpyâ€•and entropyâ€driven models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 62-70.	14.6	34
14	Computer simulation of charged hard spherocylinders. Journal of Chemical Physics, 2008, 128, 044506.	3.0	30
15	Coarse-Grained Modeling of Antibodies from Small-Angle Scattering Profiles. Journal of Physical Chemistry B, 2017, 121, 8276-8290.	2.6	30
16	A Monte Carlo simulation study of binary mixtures of charged hard spherocylinders and charged hard spheres. Chemical Physics Letters, 2009, 470, 67-71.	2.6	22
17	Directed self-assembly of spherical caps via confinement. Soft Matter, 2013, 9, 9153.	2.7	22
18	Orientational ordering and phase behaviour of binary mixtures of hard spheres and hard spherocylinders. Journal of Chemical Physics, 2015, 143, 044906.	3.0	21

#	Article	IF	Citations
19	Computer simulation of charged hard spherocylinders at low temperatures. Molecular Physics, 2011, 109, 27-36.	1.7	20
20	Liquid Adsorption of Organic Compounds on Hematite Î±-Fe2O3 Using ReaxFF. Langmuir, 2017, 33, 11257-11263.	3.5	18
21	Demixing, surface nematization, and competing adsorption in binary mixtures of hard rods and hard spheres under confinement. Journal of Chemical Physics, 2018, 148, 164701.	3.0	13
22	Liquid crystalline behavior of a coarse-grained model of shape-persistent macrocycles with flexible attractive chains. Soft Matter, 2011, 7, 1694-1701.	2.7	12
23	Degenerate crystals from colloidal dimers under confinement. Soft Matter, 2014, 10, 9729-9738.	2.7	12
24	Nanorings in planar confinement: the role of repulsive surfaces on the formation of lacuna smectics. Molecular Physics, 2018, 116, 2901-2910.	1.7	11
25	Liquid crystalline and antinematic behavior of shape-persistent macrocycles from molecular-dynamics simulations. Physical Review E, 2009, 80, 061702.	2.1	10
26	Assessment of the Wolf method using the Stillingerâ€"Lovett sum rules: From strong electrolytes to weakly charged colloidal dispersions. Journal of Chemical Physics, 2020, 153, 234901.	3.0	9
27	Engineering porous two-dimensional lattices via self-assembly of non-convex hexagonal platelets. Molecular Systems Design and Engineering, 2020, 5, 376-384.	3.4	8
28	Competitive Adsorption of a Multifunctional Amine and Phenol Surfactant with Ethanol on Hematite from Nonaqueous Solution. Journal of Physical Chemistry B, 2019, 123, 1375-1383.	2.6	7
29	Analytic expressions for the isosteric heat of adsorption from adsorption isotherm models and twoâ€dimensional <scp>SAFTâ€VR</scp> equation of state. AIChE Journal, 2021, 67, e17186.	3.6	7
30	Phase behaviour and gravity-directed self assembly of hard convex spherical caps. Soft Matter, 2017, 13, 2085-2098.	2.7	5
31	Macroscopic chiral symmetry breaking in monolayers of achiral nonconvex platelets. Soft Matter, 2017, 13, 8618-8624.	2.7	5
32	Predicting filtration of needle-like crystals: A Monte Carlo simulation study of polydisperse packings of spherocylinders. Chemical Engineering Science, 2021, 230, 116151.	3.8	3
33	Properties of a hard-core Yukawa fluid in a uniform gravitational field obtained by a hybrid DFT-Monte Carlo method. Molecular Physics, 2011, 109, 1467-1476.	1.7	2
34	Photonic mesophases from cut rod rotators. Journal of Applied Physics, 2016, 119, 023110.	2.5	1
35	Plastic fluctuations in empty crystals formed by cubic wireframe particles. Physical Review Materials, 2018, 2, .	2.4	1
36	Structural relaxation dynamics of colloidal nanotrimers. Physical Review E, 2022, 106, .	2.1	1