Alejandro Gil-Villegas

List of Publications by Year
in descending order

84 papers	3,802 citations	201575 27 h-index	123376 61 g-index
86 all docs	86 docs citations	86 times ranked	1538 citing authors

#	Article	IF	Citations
1	Equivalence between Wolf and Yukawa non-homogeneous fluids in a gravitational field. Molecular Physics, 2022, 120, .	0.8	1
2	Long-time relaxation dynamics in nematic and smectic liquid crystals of soft repulsive colloidal rods. Physical Review E, 2022, 105, 014703.	0.8	2
3	Spontaneous Pattern Growth on Chocolate Surface: Simulations and Experiments. Frontiers in Physics, 2021, 9, .	1.0	1
4	Confined Quantum Hard Spheres. Entropy, 2021, 23, 775.	1.1	0
5	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.	1.8	7
6	Wertheim Model for Quantum Associating Hard Spheres. Journal of Chemical & Engineering Data, 2020, 65, 5933-5937.	1.0	1
7	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.	1.2	9
8	Monte Carlo simulation of an associating fluid model to describe polymerization in polycaprolactone diols: The role of attractive sites of variable range. Journal of Molecular Liquids, 2019, 294, 111587.	2.3	0
9	Modelling adsorption using an augmented two-dimensional statistical associating fluid theory: 2D-SAFT-VR Mie. Molecular Physics, 2019, 117, 3770-3782.	0.8	7
10	The radial and background distribution functions of Quantum Hard Spheres. Journal of Molecular Liquids, 2019, 279, 88-93.	2.3	2
11	Theoretical equations of state for a charged fluid. Journal of Chemical Physics, 2019, 150, 144507.	1.2	9
12	Semiclassical SAFT-VR-2D modeling of adsorption selectivities for binary mixtures of hydrogen and methane adsorbed onto MOFs. Fluid Phase Equilibria, 2018, 462, 153-171.	1.4	6
13	Microcanonical-ensemble computer simulation of the high-temperature expansion coefficients of the Helmholtz free energy of a square-well fluid. Molecular Physics, 2018, 116, 351-360.	0.8	26
14	Molecular thermodynamics of a quantum Lennard-Jones fluid using an effective Mie potential and the SAFT-VR-Mie approach. Molecular Physics, 2018, 116, 3425-3433.	0.8	6
15	Computer simulation of effective potentials for generalized Boltzmann-Gibbs statistics. Journal of Molecular Liquids, 2017, 248, 364-369.	2.3	9
16	Predicting adsorption isotherms for methanol and water onto different surfaces using the SAFT-VR-2D approach and molecular simulation. Fluid Phase Equilibria, 2017, 449, 207-216.	1.4	13
17	Assessment by Monte Carlo computer simulations of the phase behavior of hard spherocylinders confined within cylindrical cavities. Journal of Chemical Physics, 2017, 147, 234902.	1.2	3
18	Monte Carlo characterization of the GammaMed HDR Plus Ir-192 brachytherapy source. Biomedical Physics and Engineering Express, 2016, 2, 015017.	0.6	1

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19	Molecular thermodynamics of quantum square-well fluids using a path-integral perturbation theory. Molecular Physics, 2016, 114, 2700-2716.	0.8	9
20	Microcanonical ensemble simulation method applied to discrete potential fluids. Physical Review E, 2015, 92, 033303.	0.8	8
21	Monte Carlo computer simulation of sedimentation of charged hard spherocylinders. Journal of Chemical Physics, 2014, 141, 044905.	1.2	11
22	Theoretical modelling of adsorption of hydrogen onto graphene, MOFs and other carbon-basedÂsubstrates. Molecular Physics, 2014, 112, 2330-2338.	0.8	14
23	Dosimetric study of surface applicators of HDR brachytherapy GammaMed Plus equipment. , 2014, , .		1
24	Predicting reactive equilibria of biodiesel's fatty-acid-methyl-esters compounds. Journal of Molecular Liquids, 2013, 185, 8-12.	2.3	8
25	Monte Carlo simulation of flexible trimers: From square well chains to amphiphilic primitive models. Journal of Chemical Physics, 2013, 139, 114901.	1.2	9
26	Generalized information entropies depending only on the probability distribution. Physical Review E, 2013, 88, 062146.	0.8	19
27	Computer simulation of liquid-vapor coexistence of confined quantum fluids. Journal of Chemical Physics, 2013, 139, 184505.	1.2	18
28	Semiclassical approach to model quantum fluids using the statistical associating fluid theory for systems with potentials of variable range. Journal of Chemical Physics, 2012, 136, 184506.	1.2	16
29	Anomalous columnar order of charged colloidal platelets. Journal of Chemical Physics, 2012, 136, 034901.	1.2	17
30	Computer simulation of sedimentation of ionic systems using the Wolf method. Journal of Chemical Physics, 2012, 136, 154507.	1.2	18
31	Evaluation of the pressure tensor and surface tension for molecular fluids with discontinuous potentials using the volume perturbation method. Journal of Chemical Physics, 2012, 137, 204104.	1.2	18
32	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.	0.8	2
33	Computer simulation of charged hard spherocylinders at low temperatures. Molecular Physics, 2011, 109, 27-36.	0.8	20
34	Modelling Adsorption Isotherms of Binary Mixtures of Carbon Dioxide, Methane and Nitrogen. Adsorption Science and Technology, 2011, 29, 59-70.	1.5	17
35	Predicting thermophysical properties of biodiesel fuel blends using the SAFT-VR approach. Fluid Phase Equilibria, 2011, 306, 124-128.	1.4	24
36	Molecular thermodynamics of biodiesel fuel compounds. Fluid Phase Equilibria, 2010, 293, 182-189.	1.4	21

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37	A Monte Carlo simulation study of binary mixtures of charged hard spherocylinders and charged hard spheres. Chemical Physics Letters, 2009, 470, 67-71.	1.2	22
38	Predicting adsorption isotherms of asphaltenes in porous materials. Fluid Phase Equilibria, 2009, 286, 113-119.	1.4	51
39	Magnetic Properties of Synthetic Eumelaninâ€"Preliminary Results^{â€}. Photochemistry and Photobiology, 2008, 84, 627-631.	1.3	10
40	Pattern formation and Interactions of Like-Charged Colloidal Particles at the Airâ^•Water Interface. AIP Conference Proceedings, 2008, , .	0.3	1
41	Computer simulation of charged hard spherocylinders. Journal of Chemical Physics, 2008, 128, 044506.	1.2	30
42	Molecular Thermodynamics of Adsorption using Discrete-Potential Systems. Oil and Gas Science and Technology, 2008, 63, 329-341.	1.4	30
43	Predicting adsorption isotherms using a two-dimensional statistical associating fluid theory. Journal of Chemical Physics, 2007, 126, 074707.	1.2	48
44	Excluded volume of hard cylinders of variable aspect ratio. Molecular Simulation, 2007, 33, 505-515.	0.9	21
45	Predicting the Phase Diagram of Two-Dimensional Colloidal Systems with Long-Range Interactionsâ€. Journal of Physical Chemistry B, 2006, 110, 22230-22236.	1.2	14
46	Predicting the Phase Behavior of Nitrogen +n-Alkanes for Enhanced Oil Recovery from the SAFT-VR Approach:Â Examining the Effect of the Quadrupole Moment. Journal of Physical Chemistry B, 2006, 110, 24083-24092.	1.2	43
47	Monte Carlo simulations of primitive models for ionic systems using the Wolf method. Molecular Physics, 2006, 104, 1475-1486.	0.8	48
48	Computer simulation of magnetic properties of human blood. Chemical Physics Letters, 2006, 432, 548-552.	1.2	7
49	Thermodynamic and structural properties of confined discrete-potential fluids. Journal of Chemical Physics, 2006, 125, 204715.	1.2	26
50	Asphaltene precipitation in crude oils: Theory and experiments. AICHE Journal, 2004, 50, 2552-2570.	1.8	245
51	Molecular View of the Asphaltene Aggregation Behavior in Asphalteneâ^'Resin Mixtures. Energy & Fuels, 2003, 17, 1100-1108.	2.5	69
52	Properties of Confined Square-well Fluids using the Gibbs Ensemble Simulation Technique. Molecular Simulation, 2003, 29, 345-356.	0.9	14
53	Orientational structure of dipolar hard-spherical colloids. Physical Review E, 2002, 65, 031401.	0.8	8
54	Computer simulations of confined colloidal systems at the air/water interface. Journal of Physics Condensed Matter, 2002, 14, 4795-4804.	0.7	20

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55	Predicting the Phase Diagram of a Liquid Crystal Using the Convex Peg Model and the Semiempirical PM3 Method. Journal of Physical Chemistry A, 2002, 106, 10342-10349.	1.1	21
56	Orthogonal functions invariant for the time-dependent harmonicÂoscillator. Physics Letters, Section A: General, Atomic and Solid State Physics, 2002, 292, 243-245.	0.9	22
57	A statistical associating fluid theory for electrolyte solutions (SAFT-VRE). Molecular Physics, 2001, 99, 531-546.	0.8	84
58	Perturbation theory for mixtures of discrete potential fluids. Molecular Physics, 2001, 99, 703-710.	0.8	47
59	Simulation study of the phase behavior of a primitive model for thermotropic liquid crystals: Rodlike molecules with terminal dipoles and flexible tails. Journal of Chemical Physics, 2000, 112, 9092-9104.	1.2	44
60	Gibbs ensemble computer simulation and SAFT-VR theory of non-conformal square-well monomerâ€“dimer mixtures. Chemical Physics Letters, 1999, 303, 27-36.	1.2	27
61	SAFT-VRE:Â Phase Behavior of Electrolyte Solutions with the Statistical Associating Fluid Theory for Potentials of Variable Range. Journal of Physical Chemistry B, 1999, 103, 10272-10281.	1.2	199
62	The thermodynamics of molecules with discrete potentials. Molecular Physics, 1999, 97, 1225-1232.	0.8	62
63	An analytical equation of state for chain molecules formed from Yukawa segments. Journal of Chemical Physics, 1999, 111, 8659-8665.	1.2	65
64	The thermodynamics of heteronuclear molecules formed from bonded square-well (BSW) segments using the SAFT-VR approach. Molecular Physics, 1999, 97, 551-558.	0.8	66
65	Title is missing!. International Journal of Thermophysics, 1998, 19, 675-686.	1.0	80
66	Computer simulation of dipolar liquid crystals. Journal of Molecular Liquids, 1998, 76, 171-181.	2.3	20
67	The effect of dipolar interactions on the liquid crystalline phase transitions of hard spherocylinders with central longitudinal dipoles. Molecular Physics, 1998, 95, 657-673.	0.8	63
68	Predicting the High-Pressure Phase Equilibria of Binary Mixtures of Perfluoro-n-alkanes +n-Alkanes Using the SAFT-VR Approach. Journal of Physical Chemistry B, 1998, 102, 8060-8069.	1.2	115
69	Predicting the High-Pressure Phase Equilibria of Binary Mixtures of n-Alkanes Using the SAFT-VR Approach. International Journal of Thermophysics, 1998, 19, 1511-1522.	1.0	60
70	Predicting the High-Pressure Phase Equilibria of Methane +n-Hexane Using the SAFT-VR Approach. Journal of Physical Chemistry B, 1998, 102, 4183-4188.	1.2	78
71	Prediction of Phase Equilibria for Refrigerant Mixtures of Difluoromethane (HFC-32), 1,1,1,2-Tetrafluoroethane (HFC-134a), and Pentafluoroethane (HFC-125a) Using SAFT-VR. Journal of Physical Chemistry B, 1998, 102, 7632-7639.	1.2	77
72	Phase equilibria of a square-well monomer-dimer mixture: Gibbs ensemble computer simulation and statistical associating fluid theory for potentials of variable range. Physical Review E, 1998, 57, 2035-2044.	0.8	20

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73	The thermodynamics of mixtures and the corresponding mixing rules in the SAFT-VR approach for potentials of variable range. Molecular Physics, 1998, 93, 241-252.	0.8	323
74	Reaction-field and Ewald summation methods in Monte Carlo simulations of dipolar liquid crystals. Molecular Physics, 1997, 92, 723-734.	0.8	61
75	Statistical associating fluid theory for chain molecules with attractive potentials of variable range. Journal of Chemical Physics, 1997, 106, 4168-4186.	1.2	932
76	Chain and ring structures in smectic phases of molecules with transverse dipoles. Chemical Physics Letters, 1997, 269, 441-447.	1.2	70
77	Deviations from corresponding-states behavior in the vapor-liquid equilibrium of the square-well fluid. Fluid Phase Equilibria, 1996, 119, 97-112.	1.4	72
78	The liquid-crystalline phase behaviour of hard spherocylinders with terminal point dipoles. Journal of Physics Condensed Matter, 1996, 8, 9649-9655.	0.7	55
79	Thermodynamics of fluids obtained by mapping the collision properties. Physical Review E, 1996, 53, 2326-2336.	0.8	25
80	Collision Diameters, Interaction Potentials, and Virial Coefficients of Small Quasi-Spherical Molecules. The Journal of Physical Chemistry, 1996, 100, 9104-9115.	2.9	18
81	Thickness dependence of the phase conjugate signal of amorphous selenium thin films. Optics Communications, 1995, 119, 154-158.	1.0	3
82	Structure of variable-width square-well fluids from the reference hypernetted chain equation. Molecular Physics, 1995, 86, 857-864.	0.8	17
83	Collision frequencies and mean collision parameters in the Lennard-Jones system. Molecular Physics, 1992, 77, 223-238.	0.8	6
84	Propagation of rays in a duct with a radially variable refractive index: First integral solutions for gaussian profiles. Optics Communications, 1988, 69, 105-107.	1.0	9