Giuseppe B Suffritti

List of Publications by Year
in descending order

94 papers	2,338 citations	218677 26 h-index	223800 46 g-index
95 all docs	95 docs citations	95 times ranked	1494 citing authors

#	Article	IF	Citations
1	Structure and Dynamics of Zeolites Investigated by Molecular Dynamics. Chemical Reviews, 1997, 97, 2845-2878.	47.7	250
2	Molecular dynamics studies on zeolites. 4. Diffusion of methane in silicalite. The Journal of Physical Chemistry, 1990, 94, 4329-4334.	2.9	168
3	Force Field for Molecular Dynamics Computations in Flexible ZIF-8 Framework. Journal of Physical Chemistry C, 2012, 116, 933-938.	3.1	146
4	Behavior of Water in the Hydrophobic Zeolite Silicalite at Different Temperatures. A Molecular Dynamics Study. Journal of Physical Chemistry B, 2003, 107, 4426-4436.	2.6	102
5	Application of the Wolf method for the evaluation of Coulombic interactions to complex condensed matter systems: Aluminosilicates and water. Journal of Chemical Physics, 2001, 114, 7980-7988.	3.0	83
6	Latticeâ€dynamical calculations on some rigid organic molecules. Journal of Chemical Physics, 1973, 59, 5088-5101.	3.0	73
7	Diffusion Anomaly as a Function of Molecular Length of Linear Molecules:Â Levitation Effect. Journal of the American Chemical Society, 2003, 125, 7116-7123.	13.7	64
8	Molecular dynamics studies on zeolites. II: A simple model for silicates applied to anhydrous natrolite. Zeolites, 1987, 7, 522-527.	0.5	61
9	NMR studies of carbon dioxide and methane self-diffusion in ZIF-8 at elevated gas pressures. Adsorption, 2012, 18, 359-366.	3.0	59
10	Molecular-dynamics calculations of thermodynamic properties of metastable alloys. Physical Review B, 1997, 55, 837-842.	3.2	57
11	A comment on the flexibility of framework in molecular dynamics simulations of zeolites. Microporous and Mesoporous Materials, 2009, 125, 160-168.	4.4	54
12	Diffusion of Water in Zeolites NaX and NaY Studied by Quasi-Elastic Neutron Scattering and Computer Simulation. Journal of Physical Chemistry C, 2009, 113, 12373-12379.	3.1	53
13	Dynamical behavior of one-dimensional water molecule chains in zeolites: Nanosecond time-scale molecular dynamics simulations of bikitaite. Journal of Chemical Physics, 2004, 120, 9233-9244.	3.0	51
14	Molecular dynamics investigation of the diffusion of methane in a cubic symmetry zeolite of type ZK4. Chemical Physics Letters, 1994, 223, 355-362.	2.6	48
15	Dynamical Properties of Confined Water Nanoclusters: Simulation Study of Hydrated Zeolite NaA: Structural and Vibrational Properties. ACS Nano, 2008, 2, 1603-1614.	14.6	48
16	Statics and Dynamics of Ethane Molecules in AlPO4-5:Â A Molecular Dynamics Simulation Study. Journal of the American Chemical Society, 2001, 123, 5069-5074.	13.7	44
17	The behaviour of water confined in zeolites: molecular dynamics simulations versus experiment. Journal of Physics Condensed Matter, 2010, 22, 284106.	1.8	41
18	â€œTwo-stepâ€•model of molecular diffusion in silicalite. Journal of Chemical Physics, 1999, 110, 1163-1172.	3.0	40

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19	Molecular dynamics studies on zeolites. Part 5.â€"Discussion of the structural changes of silicalite. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1657-1663.	1.7	37
20	Atom pair potential for molecular dynamics simulations of structural and dynamical properties of aluminosilicates: test on silicalite and anhydrous Na-A and Ca-A zeolites and comparison with experimental data. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 525.	1.7	37
21	A molecular dynamics study of diffusion of methane in silicalite molecular sieve at high dilution. Chemical Physics Letters, 1992, 191, 553-560.	2.6	36
22	Diffusion and vibrational relaxation of a diatomic molecule in the pore network of a pure silica zeolite: A molecular dynamics study. Journal of Chemical Physics, 1996, 105, 5586-5594.	3.0	36
23	Simulation of growth of Ni-Zr interfacial amorphous regions under nonequilibrium conditions. Physical Review B, 1994, 50, 2850-2857.	3.2	33
24	Thermodynamic functions for crystals of â€œrigidâ€•hydrocarbon molecules: A derivation via the Born-von Karman procedure. Chemical Physics, 1975, 8, 136-146.	1.9	32
25	Molecular dynamics simulation of anomalous diffusion of one-dimensional water molecule chains in Li-ABW zeolite. Microporous and Mesoporous Materials, 2005, 86, 166-175.	4.4	32
26	Diffusion of Water in Zeolites Na A and NaCa A: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2010, 114, 18612-18621.	3.1	26
27	Estimation of Partial Charges in Small Zeolite Imidazolate Frameworks from Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2011, 7, 1575-1582.	5.3	25
28	Use of anisotropic atom-atom potential functions in lattice-dynamical calculations for solid nitrogen. Molecular Physics, 1978, 35, 1659-1667.	1.7	24
29	Understanding Diffusion in Confined Systems:â€‰ Methane in a ZK4 Molecular Sieve. A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2005, 109, 18081-18087.	2.6	23
30	Amorphization of calcined LTA zeolites at high pressure: a computational study. Microporous and Mesoporous Materials, 2004, 69, 127-134.	4.4	22
31	Development and Optimization of a New Force Field for Flexible Aluminosilicates, Enabling Fast Molecular Dynamics Simulations on Parallel Architectures. Journal of Physical Chemistry C, 2013, 117, 503-509.	3.1	22
32	A Lattice-Gas Cellular Automaton to Model Diffusion in Restricted Geometries. Journal of Physical Chemistry B, 2006, 110, 13554-13559.	2.6	21
33	Partial Charges in Periodic Systems: Improving Electrostatic Potential (ESP) Fitting via Total Dipole Fluctuations and Multiframe Approaches. Journal of Chemical Theory and Computation, 2015, 11, 3829-3843.	5.3	21
34	Application of the two-step model to the diffusion of linear diatomic and triatomic molecules in silicalite. Physical Chemistry Chemical Physics, 2000, 2, 1455-1463.	2.8	19
35	Fractional diffusion interpretation of simulated single-file systems in microporous materials. Physical Review E, 2006, 74, 051112.	2.1	19
36	Lattice dynamics in crystals of â€˜rigidâ€™ hydrocarbons. Chemical Physics Letters, 1973, 20, 23-28.	2.6	17

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37	An effective harmonic potential for aluminophosphate molecular sieves: application to AlPO4-5. Microporous and Mesoporous Materials, 2001, 42, 103-111.	4.4	17
38	Thermal parameters of 11,11-dimethyltricyclo [4,4,1,01,6] undeca-2,4,7,9-tetraene: A lattice-dynamical discussion. Chemical Physics Letters, 1974, 26, 301-304.	2.6	16
39	Lattice-dynamical evaluation of cell parameters of some hydrocarbons at various temperatures. Chemical Physics Letters, 1975, 35, 17-20.	2.6	16
40	Lattice-Dynamical calculations on some aromatic fluoro derivatives. Chemical Physics Letters, 1976, 39, 14-18.	2.6	16
41	A potential for molecular dynamics simulations of structural and dynamic properties of hydrate aluminosilicates. Materials Chemistry and Physics, 1991, 29, 357-367.	4.0	16
42	An implemented potential of non-rigid water molecules for molecular dynamics simulations. Chemical Physics Letters, 1986, 127, 456-461.	2.6	15
43	Molecular Dynamics Simulation Study of Superhydrated Perdeuterated Natrolite Using a New Interaction Potential Model. Journal of Physical Chemistry B, 2006, 110, 7513-7518.	2.6	15
44	Lattice-dynamical calculations on solid nitrogen. Chemical Physics Letters, 1976, 40, 210-214.	2.6	13
45	Introducing a Cellular Automaton as an Empirical Model to Study Static and Dynamic Properties of Molecules Adsorbed in Zeolites. Journal of Physical Chemistry B, 2008, 112, 12444-12452.	2.6	13
46	Water Adsorbed in AlPO₄-5 and SSZ-24 Studied by Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2012, 116, 11100-11109.	3.1	13
47	Peculiar Structure of Water in Slightly Superhydrated Vermiculite Clay Studied by Carâ€“Parrinello Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2014, 118, 7923-7931.	3.1	13
48	Diffusion in tight confinement: A lattice-gas cellular automaton approach. I. Structural equilibrium properties. Journal of Chemical Physics, 2007, 126, 194709.	3.0	12
49	Molecular dynamics simulation of an activated transfer reaction in zeolites. Journal of Chemical Physics, 1999, 111, 5529-5543.	3.0	11
50	Comment on â€œDoes lattice vibration drive diffusion in zeolites?â€•[J. Chem. Phys. 114, 3776 (2001)]. Journal of Chemical Physics, 2003, 118, 3439-3440.	3.0	11
51	From thermodynamic cell models to partitioning cellular automata for diffusion in zeolites. I. Structure of the algorithm. Journal of Chemical Physics, 2009, 131, 234703.	3.0	11
52	A Grand-Canonical Monte Carlo Study of the Adsorption Properties of Argon Confined in ZIF-8: Local Thermodynamic Modeling. Journal of Physical Chemistry C, 2013, 117, 349-357.	3.1	11
53	Diffusion in tight confinement: A lattice-gas cellular automaton approach. II. Transport properties. Journal of Chemical Physics, 2007, 126, 194710.	3.0	10
54	From thermodynamic cell models to partitioning cellular automata for diffusion in zeolites. II. Static and dynamic properties. Journal of Chemical Physics, 2009, 131, 234704.	3.0	10

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55	Fast and efficient optimization of Molecular Dynamics force fields for microporous materials: Bonded interactions via force matching. Microporous and Mesoporous Materials, 2014, 197, 339-347.	4.4	10
56	Two- and N-step correlated models for the analysis of molecular dynamics trajectories of linear molecules in silicalite. Journal of Chemical Physics, 2000, 113, 7588-7592.	3.0	9
57	A classical molecular dynamics study of recombination reactions in a microporous solid. Journal of Chemical Physics, 1998, 109, 2865-2873.	3.0	8
58	Recombination Reactions and Diffusive Properties of Diatomic Molecules in Two Different Microporous Structures:â€‰ Silicalite and ZK4. Journal of Physical Chemistry B, 1999, 103, 8141-8152.	2.6	8
59	A molecular dynamics study and molecular level explanation of pressure dependence of ionic conductivity of potassium chloride in water. Physical Chemistry Chemical Physics, 2011, 13, 10877.	2.8	8
60	Speeding up simulation of diffusion in zeolites by a parallel synchronous kinetic Monte Carlo algorithm. Physical Review E, 2011, 83, 056705.	2.1	8
61	Simulation study of CO2 adsorption properties in small Zeolite Imidazolate Frameworks. Chemical Physics Letters, 2013, 580, 99-102.	2.6	8
62	Water Nanoconfined in Clays: The Structure of Na Vermiculite Revisited by Ab Initio Simulations. Journal of Physical Chemistry C, 2013, 117, 15583-15592.	3.1	8
63	Molecular dynamics simulations of diffusion in a cubic symmetry zeolite. Studies in Surface Science and Catalysis, 1994, , 2107-2113.	1.5	7
64	High-temperature dynamic behavior in bulk liquid water: A molecular dynamics simulation study using the OPC and TIP4P-Ew potentials. Frontiers of Physics, 2018, 13, 1.	5.0	7
65	Comment on â€œHigh-Accuracy Estimation of â€˜Slowâ€™ Molecular Diffusion Rates in Zeolite Nanopores, Based on Free Energy Calculations at an Ultrahigh Temperatureâ€• Journal of Physical Chemistry C, 2008, 112, 17030-17031.	3.1	6
66	A study of the pressure-induced reversible amorphization of Xe containing-LTA zeolites by energy minimization technique. Microporous and Mesoporous Materials, 2009, 123, 30-38.	4.4	6
67	The central cell model: A mesoscopic hopping model for the study of the displacement autocorrelation function. Journal of Chemical Physics, 2011, 134, 184109.	3.0	6
68	Computer simulations of dynamic crossover phenomena in nanoconfined water. Journal of Physics Condensed Matter, 2012, 24, 064110.	1.8	6
69	A theoretical investigation on the role of solvent in solvolytic reactions. Part 5. Fluoromethane in methane. Journal of the Chemical Society Perkin Transactions II, 1983, , 997.	0.9	5
70	The behavior of silicalite-1 under high pressure conditions studied by computational simulation. Structural Chemistry, 2013, 24, 909-915.	2.0	5
71	A method for correcting empirical potentials. Application to water molecule.. Computational and Theoretical Chemistry, 1985, 120, 201-206.	1.5	4
72	Effective interactions in multisite cells for adsorption in microporous materials. Journal of Chemical Physics, 2009, 130, 164701.	3.0	4

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73	Computational research on memory effects in AlPO4-5 nanoporous material. Journal of Physics and Chemistry of Solids, 2012, 73, 797-802.	4.0	4
74	Synchronous equilibrium model for the diffusion of mutually exclusive particles in a heterogeneous lattice of adsorption sites. Physical Review E, 2013, 87, 063306.	2.1	4
75	Distributions of single-molecule properties as tools for the study of dynamical heterogeneities in nanoconfined water. Journal of Physics Condensed Matter, 2014, 26, 155103.	1.8	4
76	The interplay between dynamic heterogeneities and structure of bulk liquid water: A molecular dynamics simulation study. Journal of Chemical Physics, 2015, 142, 244507.	3.0	4
77	Modelling diffusion in zeolites with cellular automata. Studies in Surface Science and Catalysis, 2008, 174, 701-704.	1.5	3
78	A parallelizable block cellular automaton for the study of diffusion of binary mixtures containing CO2 in microporous materials. Journal of Chemical Physics, 2011, 135, 124110.	3.0	3
79	Conciliating synchronicity with spatial discretization, exclusion, interactions, and detailed balance. Physical Review E, 2013, 88, 062114.	2.1	3
80	Coarse-Graining of Adsorption in Microporous Materials: Relation between Occupancy Distributions and Local Partition Functions. Journal of Physical Chemistry C, 2014, 118, 28711-28719.	3.1	3
81	A Combined Energy-Force Fitting Procedure to Develop DFT-Based Force Fields. Journal of Physical Chemistry C, 2016, 120, 26309-26319.	3.1	3
82	Reverse MÃ¶ssbauer effect as a possible source of â€œhotâ€•molecules absorbed in crystalline solids at low temperature. Journal of Chemical Physics, 2016, 145, 094110.	3.0	3
83	Derivation of a quotient group in symmetry operations. Computers & Chemistry, 1977, 1, 215-220.	1.2	2
84	Chemical potential evaluation in NVT lattice-gas simulations. Journal of Chemical Physics, 2012, 137, 154106.	3.0	2
85	A coarse-grained method based on the analysis of short molecular dynamics trajectories for the simulation of non-Markovian dynamics of molecules adsorbed in microporous materials. Journal of Chemical Physics, 2014, 141, 074109.	3.0	2
86	A network of discrete events for the representation and analysis of diffusion dynamics. Journal of Chemical Physics, 2015, 143, 184115.	3.0	2
87	Improving the acceptance in Monte Carlo simulations: Sampling through intermediate states. Journal of Computational Physics, 2015, 295, 556-568.	3.8	2
88	InfiniCharges: A tool for generating partial charges via the simultaneous fit of multiframe electrostatic potential (ESP) and total dipole fluctuations (TDF). Computer Physics Communications, 2016, 200, 190-198.	7.5	2
89	Reverse MÃ¶ssbauer effect as a possible source of â€œhotâ€•protons in hydrogen absorbing metals. International Journal of Hydrogen Energy, 2018, 43, 1725-1735.	7.1	2
90	Combining off-lattice Monte Carlo and cellular automata for the simulation of hard-sphere systems. Physical Review E, 2014, 90, 023307.	2.1	1

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91	A lattice dynamics study of ZK-4 microporous material under different temperature and pressure conditions. Microporous and Mesoporous Materials, 2016, 226, 191-200.	4.4	1
92	Computational Studies on the Effects of Pressure and Temperature on Zeolite Framework Structures. Advanced Science Letters, 2017, 23, 5824-5827.	0.2	1
93	Thermodynamics of the one-dimensional parallel Kawasaki model: Exact solution and mean-field approximations. Physical Review E, 2014, 90, 022118.	2.1	0
94	The influence of the reverse MÃ¶ssbauer effect on diffusion and desorption of hydrogen absorbed in metals. International Journal of Hydrogen Energy, 2019, 44, 18255-18264.	7.1	0