Estela Blaisten-Barojas

List of Publications by Year
in descending order

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100 papers	1,661 citations	331259 21 h-index	329751 37 g-index
106 all docs	106 docs citations	106 times ranked	1226 citing authors

#	Article	IF	Citations
1	Theoretical study on a reaction pathway of Zieglerâ€“Nattaâ€type catalysis. Journal of Chemical Physics, 1978, 68, 2337-2351.	1.2	118
2	Molecular-dynamics simulation of silicon clusters. Physical Review B, 1986, 34, 3910-3916.	1.1	110
3	Structure and dynamics of alkali-metal clusters and fission of highly charged clusters. Physical Review B, 1998, 57, 15519-15532.	1.1	87
4	Magnetic and electronic properties of rhodium clusters. Physical Review A, 1998, 58, 2196-2202.	1.0	72
5	Development of a First-Principles Many-Body Potential for Beryllium. Physical Review Letters, 1988, 61, 1477-1480.	2.9	65
6	Properties of Silicon Nanoparticles:Â A Molecular Dynamics Study. The Journal of Physical Chemistry, 1996, 100, 14856-14864.	2.9	63
7	Density functional theory study of the structure and energetics of negatively charged oligopyrroles. International Journal of Quantum Chemistry, 2011, 111, 2295-2305.	1.0	56
8	Melting and freezing of Lennard-Jones clusters on a surface. Physical Review B, 1987, 36, 8447-8455.	1.1	49
9	Concentration dependence of structural and dynamical quantities in colloidal aggregation: Computer simulations. Physical Review E, 1996, 54, 5456-5462.	0.8	49
10	Machine learning approach for structure-based zeolite classification. Microporous and Mesoporous Materials, 2009, 117, 339-349.	2.2	49
11	Phenomenological model of melting in Lennard-Jones clusters. Physical Review B, 1989, 40, 4749-4759.	1.1	42
12	Many-body potential and structure for rhodium clusters. Journal of Chemical Physics, 2000, 112, 2301-2307.	1.2	39
13	Electronic structure of calcium clusters. Physical Review A, 2001, 63, .	1.0	37
14	Identifying Zeolite Frameworks with a Machine Learning Approach. Journal of Physical Chemistry C, 2009, 113, 21721-21725.	1.5	36
15	Molecular-dynamics study of cluster growth by cluster-cluster collisions. Physical Review B, 1992, 45, 4403-4408.	1.1	35
16	Theory of atomic diffusion in cubic crystals with impurities based on the correlated-walks theory. Physical Review B, 1980, 22, 1638-1644.	1.1	32
17	Structure function and fractal dimension of diffusion-limited colloidal aggregates. Physical Review E, 1998, 57, 4520-4527.	0.8	29
18	Effects of three-body interactions on the structure of clusters. Surface Science, 1985, 156, 548-555.	0.8	27

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19	Energetics, structure, and charge distribution of reduced and oxidized n-pyrrole oligomers: A density functional approach. Journal of Chemical Physics, 2008, 129, 164903.	1.2	27
20	Strontium clusters: Many-body potential, energetics, and structural transitions. Journal of Chemical Physics, 2001, 115, 3640-3646.	1.2	25
21	Energetics and Vibrational Analysis of Methyl Salicylate Isomers. Journal of Physical Chemistry A, 2009, 113, 10385-10390.	1.1	23
22	Studies on the problem of small metallic particles. I. â€" Spectrum fluctuations in a two-dimensional model and the associated specific heat. Annals of Physics, 1977, 107, 95-109.	1.0	18
23	Exploring with Molecular Dynamics the Structural Fate of PLGA Oligomers in Various Solvents. Journal of Physical Chemistry B, 2019, 123, 10233-10244.	1.2	18
24	Effect of three-body interactions on the early stages of atomic cluster growth. Chemical Physics Letters, 1986, 124, 84-89.	1.2	17
25	Energetics and bonding in beryllium metallized carbon clusters. Computational and Theoretical Chemistry, 2007, 824, 39-47.	1.5	17
26	Framework-Type Determination for Zeolite Structures in the Inorganic Crystal Structure Database. Journal of Physical and Chemical Reference Data, 2010, 39, .	1.9	17
27	An application of Green's functions to the study of the vibration-translation coupling of trapped oscillators in a linear chain. International Journal of Quantum Chemistry, 1973, 7, 195-213.	1.0	16
28	Study of a Lorentzâ€gas based on correlated walks. Journal of Chemical Physics, 1980, 73, 4569-4576.	1.2	16
29	On the Concentration Dependence of the Cluster Fractal Dimension in Colloidal Aggregation. Journal of Sol-Gel Science and Technology, 1999, 15, 119-127.	1.1	16
30	Cluster-cluster aggregation in binary mixtures. Physical Review E, 2000, 61, 550-556.	0.8	16
31	Role of threeâ€body interactions in trimer binding. Journal of Chemical Physics, 1977, 67, 4701-4705.	1.2	15
32	Monte Carlo study of oligopyrroles in condensed phases. Journal of Chemical Physics, 2010, 133, 034905.	1.2	15
33	Theoretical investigation of the photophysics of methyl salicylate isomers. Journal of Chemical Physics, 2011, 135, 164306.	1.2	15
34	Non-additive interactions in liquid helium solvent effects. Molecular Physics, 1979, 37, 599-606.	0.8	14
35	Helixâ€“coil transition of polypeptides on the basis of correlated walks. Journal of Chemical Physics, 1981, 75, 3097-3102.	1.2	14
36	Pressure induced transitions in calcium: a tight-binding approach. Journal of Physics and Chemistry of Solids, 2003, 64, 185-192.	1.9	14

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37	Tight-binding model for calcium nanoclusters: Structural, electronic, and dynamical properties. Physical Review B, 2004, 70, .	1.1	14
38	Silicon carbide nanostructures: A tight binding approach. Journal of Chemical Physics, 2009, 130, 244704.	1.2	14
39	Lattice Thermal Conductivity in SiC Nanotubes, Nanowires and Nanofilaments: A Molecular Dynamics Study. Journal of Computational and Theoretical Nanoscience, 2011, 8, 529-534.	0.4	14
40	Molecular dynamics study of neutral and multiply charged sodium clusters. Chemical Physics Letters, 1997, 268, 331-336.	1.2	13
41	Effects of the interface between two Lennard-Jones crystals on the lattice vibrations: a molecular dynamics study. Journal of Physics Condensed Matter, 2009, 21, 345402.	0.7	13
42	The Metropolis Monte Carlo method with CUDA enabled Graphic Processing Units. Journal of Computational Physics, 2014, 258, 871-879.	1.9	13
43	Polypyrrole on graphene: A density functional theory study. Surface Science, 2018, 674, 1-5.	0.8	13
44	Molecular dynamics study of the depolymerization reaction in simple polymers. Chemical Physics Letters, 1990, 171, 499-505.	1.2	12
45	Calculation of the Magnetic Moment of Atomic Fluorine. Physical Review, 1968, 172, 44-49.	2.7	11
46	LCAOâ€“MOâ€“SCF calculation of the metalâ€“oxygen bonding in the M2O2 series: M = Li, Na, and K. Journal of Chemical Physics, 1981, 75, 787-792.	1.2	10
47	IR absorption spectrum of molecules trapped in matrices. I. The libron-phonon coupling in 1D. Journal of Physics C: Solid State Physics, 1976, 9, 3121-3139.	1.5	9
48	The vibrational line shape of diatomic adsorbates on metal clusters. Journal of Chemical Physics, 1992, 97, 862-870.	1.2	9
49	Novel Approach for Clustering Zeolite Crystal Structures. Molecular Informatics, 2010, 29, 297-301.	1.4	9
50	Bipolarons and polaron pairs in oligopyrrole dications. Computational and Theoretical Chemistry, 2012, 993, 7-12.	1.1	9
51	Density functional theory study of neutral and oxidized thiophene oligomers. Journal of Chemical Physics, 2013, 139, 184905.	1.2	9
52	Calculation of the Magnetic Moment of Atomic Oxygen. Physical Review, 1969, 177, 432-434.	2.7	8
53	Energetics and bonding in small lithiated carbon clusters. Computational and Theoretical Chemistry, 2007, 807, 163-172.	1.5	8
54	Machine learning study of the heulandite family of zeolites. Microporous and Mesoporous Materials, 2010, 130, 309-313.	2.2	8

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55	Structure, energetics and thermodynamics of PLGA condensed phases from Molecular Dynamics. Polymer, 2020, 206, 122903.	1.8	8
56	Solutions and Condensed Phases of PEG₂₀₀₀ from All-Atom Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 12892-12901.	1.2	8
57	Study of the correlated walks with reflecting walls. Journal of Chemical Physics, 1982, 76, 601-608.	1.2	7
58	Libronâ€“phonon coupling effect on the infrared absorption spectra of molecules trapped in matrices. Journal of Chemical Physics, 1985, 83, 4311-4318.	1.2	7
59	Fission of doubly ionized calcium clusters. Chemical Physics Letters, 2004, 395, 109-113.	1.2	7
60	Energetics, Structure, and Electron Detachment Spectra of Calcium and Zinc Neutral and Anion Clusters: A Density Functional Theory Study. Journal of Physical Chemistry A, 2008, 112, 11052-11060.	1.1	7
61	Vortex generation in a finitely extensible nonlinear elastic Peterlin fluid initially at rest. Engineering Reports, 2020, 2, e12135.	0.9	7
62	Solvent effects of liquid helium on He2. Molecular Physics, 1976, 31, 1941-1944.	0.8	6
63	Density functional theory study of dipicolinic acid isomers and crystalline polytypes. Computational and Theoretical Chemistry, 2011, 977, 148-156.	1.1	6
64	Electronic structure and vibrational analysis of the alkali peroxides K2O2 and Rb2O2. Chemical Physics Letters, 1984, 108, 237-240.	1.2	5
65	Failure of logarithmic oscillators to serve as a thermostat for small atomic clusters. Physical Review E, 2014, 89, 021301.	0.8	5
66	Simulating the NaK Eutectic Alloy with Monte Carlo and Machine Learning. Scientific Reports, 2019, 9, 704.	1.6	5
67	Modeling the Tertiary Structure of the Rift Valley Fever Virus L Protein. Molecules, 2019, 24, 1768.	1.7	5
68	Permeation in Gramicidin Ion Channels by Directly Estimating the Potential of Mean Force Using Brownian Dynamics Simulations. Journal of Computational and Theoretical Nanoscience, 2006, 3, 702-711.	0.4	5
69	Forecasting molecular dynamics energetics of polymers in solution from supervised machine learning. Chemical Science, 2022, 13, 7021-7033.	3.7	5
70	A correlated walk model for thermally stimulated depolarization currents in Î±â€keratin. Journal of Chemical Physics, 1982, 76, 5643-5645.	1.2	4
71	New potentials for Si2+. Chemical Physics Letters, 1988, 150, 259-262.	1.2	4
72	A cloud computing system in windows azure platform for data analysis of crystalline materials. Concurrency Computation Practice and Experience, 2013, 25, 2157-2169.	1.4	4

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73	Polyacrylamide in glycerol solutions from an atomistic perspective of the energetics, structure, and dynamics. AIP Advances, 2020, 10, .	0.6	4
74	Dependence of the specific heat on the spectrum fluctuations. Physics Letters, Section A: General, Atomic and Solid State Physics, 1977, 61, 146-148.	0.9	3
75	Two examples of electronic spectrum fluctuations in microparticles. Physics Letters, Section A: General, Atomic and Solid State Physics, 1978, 69, 142-144.	0.9	3
76	Ab initio molecular orbital study of the catalytic exchange reaction between hydrogen and sodium amide. Journal of Chemical Physics, 1979, 71, 5124.	1.2	3
77	Correlated walk model of the melting transition in small clusters. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 2351.	1.7	3
78	The helix-coil transition based on correlated walks. Ferroelectrics, 1980, 30, 299-304.	0.3	2
79	More on the melting of Lennard-Jones clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 181-183.	1.0	2
80	Nonlinear coupling between rotation and internal vibration in simple molecular systems. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 309-318.	0.6	2
81	Tight-binding Calcium Clusters from Adaptive Tempering Monte Carlo Simulation. Computing Letters, 2005, 1, 152-157.	0.5	2
82	Computational study of heat transport in compositionally disordered binary crystals. Acta Materialia, 2006, 54, 4633-4639.	3.8	2
83	Protein folding with the adaptive tempering Monte Carlo method. Molecular Simulation, 2007, 33, 577-582.	0.9	2
84	A Cheminformatics Approach for Zeolite Framework Determination. Lecture Notes in Computer Science, 2009, , 160-168.	1.0	2
85	The libronâ€“phonon coupling and the IR absorption spectra of diatomic molecules in a simple liquid. Journal of Chemical Physics, 1985, 82, 1772-1778.	1.2	1
86	Model potential for beryllium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 77-79.	1.0	1
87	Molecular Dynamics Simulation of Large Cluster Growth. Materials Research Society Symposia Proceedings, 1993, 334, 75.	0.1	1
88	Atomistic Simulation of Vapor-Phase Nanoparticle Formation. Materials Research Society Symposia Proceedings, 1994, 351, 343.	0.1	1
89	Irregular scattering of particles confined to ring-bounded cavities. Journal of Statistical Physics, 1997, 87, 137-146.	0.5	1
90	Colloidal aggregation with mobile impurities. Physical Review E, 2000, 61, 6781-6788.	0.8	1

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91	Monte Carlo Study of the Crystalline and Amorphous NaK Alloy. Procedia Computer Science, 2017, 108, 1215-1221.	1.2	1
92	Study of Solidâ€“Liquid Phase Changes of Lennard-Jones Nanoclusters by NPT Monte Carlo Simulations. Journal of Computational and Theoretical Nanoscience, 2007, 4, 529-534.	0.4	1
93	Distinctive Formation of PEG-Lipid Nanopatches onto Solid Polymer Surfaces Interfacing Solvents from Atomistic Simulation. Journal of Physical Chemistry B, 2022, 126, 1598-1608.	1.2	1
94	MOLECULAR DYNAMICS STUDY OF CLUSTER GROWTH AND POLYMER DEGRADATION. International Journal of Modern Physics B, 1992, 06, 3643-3655.	1.0	0
95	Dynamics of Nanometer SiO2 Particles and their Coalescence Characteristics. Materials Research Society Symposia Proceedings, 1994, 366, 173.	0.1	0
96	Fragmentation of Highly Charged Metallic Clusters. Materials Research Society Symposia Proceedings, 1994, 366, 341.	0.1	0
97	Modeling the Tertiary Structure of a Multi-domain Protein. , 2018, , .		0
98	Front Cover Image, Volume 2, Number 3, March 2020. Engineering Reports, 2020, 2, e12162.	0.9	0
99	Modeling oxidised polypyrrole in the condensed phase with a novel force field. Journal of Physics Condensed Matter, 2022, 34, 185701.	0.7	0
100	Structural and Dynamical Properties of Clusters on A Substrate. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1987, , 241-251.	0.2	0