# 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 | Modeling oxidised polypyrrole in the condensed phase with a novel force field. Journal of Physics Condensed Matter, 2022, 34, 185701. | 0.7 | 0 |
| 2 | 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 |
| 3 | Forecasting molecular dynamics energetics of polymers in solution from supervised machine learning. Chemical Science, 2022, 13, 7021-7033. | 3.7 | 5 |
| 4 | Solutions and Condensed Phases of PEG<sub>2000</sub> from All-Atom Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 12892-12901. | 1.2 | 8 |
| 5 | Front Cover Image, Volume 2, Number 3, March 2020. Engineering Reports, 2020, 2, e12162. | 0.9 | 0 |
| 6 | Structure, energetics and thermodynamics of PLGA condensed phases from Molecular Dynamics. Polymer, 2020, 206, 122903. | 1.8 | 8 |
| 7 | Polyacrylamide in glycerol solutions from an atomistic perspective of the energetics, structure, and dynamics. AIP Advances, 2020, 10, . | 0.6 | 4 |
| 8 | Vortex generation in a finitely extensible nonlinear elastic Peterlin fluid initially at rest. Engineering Reports, 2020, 2, e12135. | 0.9 | 7 |
| 9 | 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 |
| 10 | Simulating the NaK Eutectic Alloy with Monte Carlo and Machine Learning. Scientific Reports, 2019, 9, 704. | 1.6 | 5 |
| 11 | Modeling the Tertiary Structure of the Rift Valley Fever Virus L Protein. Molecules, 2019, 24, 1768. | 1.7 | 5 |
| 12 | Polypyrrole on graphene: A density functional theory study. Surface Science, 2018, 674, 1-5. | 0.8 | 13 |
| 13 | Modeling the Tertiary Structure of a Multi-domain Protein. , 2018, , . | | 0 |
| 14 | Monte Carlo Study of the Crystalline and Amorphous NaK Alloy. Procedia Computer Science, 2017, 108, 1215-1221. | 1.2 | 1 |
| 15 | Failure of logarithmic oscillators to serve as a thermostat for small atomic clusters. Physical Review E, 2014, 89, 021301. | 0.8 | 5 |
| 16 | The Metropolis Monte Carlo method with CUDA enabled Graphic Processing Units. Journal of Computational Physics, 2014, 258, 871-879. | 1.9 | 13 |
| 17 | Density functional theory study of neutral and oxidized thiophene oligomers. Journal of Chemical Physics, 2013, 139, 184905. | 1.2 | 9 |
| 18 | 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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| 19 | Bipolarons and polaron pairs in oligopyrrole dications. Computational and Theoretical Chemistry, 2012, 993, 7-12. | 1.1 | 9 |
| 20 | Density functional theory study of dipicolinic acid isomers and crystalline polytypes. Computational and Theoretical Chemistry, 2011, 977, 148-156. | 1.1 | 6 |
| 21 | 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 |
| 22 | 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 |
| 23 | Theoretical investigation of the photophysics of methyl salicylate isomers. Journal of Chemical Physics, 2011, 135, 164306. | 1.2 | 15 |
| 24 | Novel Approach for Clustering Zeolite Crystal Structures. Molecular Informatics, 2010, 29, 297-301. | 1.4 | 9 |
| 25 | Machine learning study of the heulandite family of zeolites. Microporous and Mesoporous Materials, 2010, 130, 309-313. | 2.2 | 8 |
| 26 | Monte Carlo study of oligopyrroles in condensed phases. Journal of Chemical Physics, 2010, 133, 034905. | 1.2 | 15 |
| 27 | Framework-Type Determination for Zeolite Structures in the Inorganic Crystal Structure Database. Journal of Physical and Chemical Reference Data, 2010, 39, . | 1.9 | 17 |
| 28 | Machine learning approach for structure-based zeolite classification. Microporous and Mesoporous Materials, 2009, 117, 339-349. | 2.2 | 49 |
| 29 | Identifying Zeolite Frameworks with a Machine Learning Approach. Journal of Physical Chemistry C, 2009, 113, 21721-21725. | 1.5 | 36 |
| 30 | Silicon carbide nanostructures: A tight binding approach. Journal of Chemical Physics, 2009, 130, 244704. | 1.2 | 14 |
| 31 | 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 |
| 32 | Energetics and Vibrational Analysis of Methyl Salicylate Isomers. Journal of Physical Chemistry A, 2009, 113, 10385-10390. | 1.1 | 23 |
| 33 | A Cheminformatics Approach for Zeolite Framework Determination. Lecture Notes in Computer Science, 2009, , 160-168. | 1.0 | 2 |
| 34 | 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 |
| 35 | 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 |
| 36 | Protein folding with the adaptive tempering Monte Carlo method. Molecular Simulation, 2007, 33, 577-582. | 0.9 | 2 |

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| 37 | Energetics and bonding in small lithiated carbon clusters. Computational and Theoretical Chemistry, 2007, 807, 163-172. | 1.5 | 8 |
| 38 | Energetics and bonding in beryllium metallized carbon clusters. Computational and Theoretical Chemistry, 2007, 824, 39-47. | 1.5 | 17 |
| 39 | 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 |
| 40 | Computational study of heat transport in compositionally disordered binary crystals. Acta Materialia, 2006, 54, 4633-4639. | 3.8 | 2 |
| 41 | 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 |
| 42 | Tight-binding Calcium Clusters from Adaptive Tempering Monte Carlo Simulation. Computing Letters, 2005, 1, 152-157. | 0.5 | 2 |
| 43 | Tight-binding model for calcium nanoclusters: Structural, electronic, and dynamical properties. Physical Review B, 2004, 70, . | 1.1 | 14 |
| 44 | Fission of doubly ionized calcium clusters. Chemical Physics Letters, 2004, 395, 109-113. | 1.2 | 7 |
| 45 | Pressure induced transitions in calcium: a tight-binding approach. Journal of Physics and Chemistry of Solids, 2003, 64, 185-192. | 1.9 | 14 |
| 46 | Electronic structure of calcium clusters. Physical Review A, 2001, 63, . | 1.0 | 37 |
| 47 | Strontium clusters: Many-body potential, energetics, and structural transitions. Journal of Chemical Physics, 2001, 115, 3640-3646. | 1.2 | 25 |
| 48 | Cluster-cluster aggregation in binary mixtures. Physical Review E, 2000, 61, 550-556. | 0.8 | 16 |
| 49 | Colloidal aggregation with mobile impurities. Physical Review E, 2000, 61, 6781-6788. | 0.8 | 1 |
| 50 | Many-body potential and structure for rhodium clusters. Journal of Chemical Physics, 2000, 112, 2301-2307. | 1.2 | 39 |
| 51 | 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 |
| 52 | Structure and dynamics of alkali-metal clusters and fission of highly charged clusters. Physical Review B, 1998, 57, 15519-15532. | 1.1 | 87 |
| 53 | Structure function and fractal dimension of diffusion-limited colloidal aggregates. Physical Review E, 1998, 57, 4520-4527. | 0.8 | 29 |
| 54 | Magnetic and electronic properties of rhodium clusters. Physical Review A, 1998, 58, 2196-2202. | 1.0 | 72 |

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| 55 | 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 |
| 56 | Irregular scattering of particles confined to ring-bounded cavities. Journal of Statistical Physics, 1997, 87, 137-146. | 0.5 | 1 |
| 57 | Molecular dynamics study of neutral and multiply charged sodium clusters. Chemical Physics Letters, 1997, 268, 331-336. | 1.2 | 13 |
| 58 | Properties of Silicon Nanoparticles:Â A Molecular Dynamics Study. The Journal of Physical Chemistry, 1996, 100, 14856-14864. | 2.9 | 63 |
| 59 | Concentration dependence of structural and dynamical quantities in colloidal aggregation: Computer simulations. Physical Review E, 1996, 54, 5456-5462. | 0.8 | 49 |
| 60 | Atomistic Simulation of Vapor-Phase Nanoparticle Formation. Materials Research Society Symposia Proceedings, 1994, 351, 343. | 0.1 | 1 |
| 61 | Dynamics of Nanometer SiO2 Particles and their Coalescence Characteristics. Materials Research Society Symposia Proceedings, 1994, 366, 173. | 0.1 | 0 |
| 62 | Fragmentation of Highly Charged Metallic Clusters. Materials Research Society Symposia Proceedings, 1994, 366, 341. | 0.1 | 0 |
| 63 | Molecular Dynamics Simulation of Large Cluster Growth. Materials Research Society Symposia Proceedings, 1993, 334, 75. | 0.1 | 1 |
| 64 | The vibrational line shape of diatomic adsorbates on metal clusters. Journal of Chemical Physics, 1992, 97, 862-870. | 1.2 | 9 |
| 65 | Molecular-dynamics study of cluster growth by cluster-cluster collisions. Physical Review B, 1992, 45, 4403-4408. | 1.1 | 35 |
| 66 | MOLECULAR DYNAMICS STUDY OF CLUSTER GROWTH AND POLYMER DEGRADATION. International Journal of Modern Physics B, 1992, 06, 3643-3655. | 1.0 | 0 |
| 67 | Molecular dynamics study of the depolymerization reaction in simple polymers. Chemical Physics Letters, 1990, 171, 499-505. | 1.2 | 12 |
| 68 | Correlated walk model of the melting transition in small clusters. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 2351. | 1.7 | 3 |
| 69 | Phenomenological model of melting in Lennard-Jones clusters. Physical Review B, 1989, 40, 4749-4759. | 1.1 | 42 |
| 70 | Model potential for beryllium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 77-79. | 1.0 | 1 |
| 71 | More on the melting of Lennard-Jones clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 181-183. | 1.0 | 2 |
| 72 | New potentials for Si2+. Chemical Physics Letters, 1988, 150, 259-262. | 1.2 | 4 |

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|---|---|---|---|
| 73 | Development of a First-Principles Many-Body Potential for Beryllium. Physical Review Letters, 1988, 61, 1477-1480. | 2.9 | 65 |
| 74 | Melting and freezing of Lennard-Jones clusters on a surface. Physical Review B, 1987, 36, 8447-8455. | 1.1 | 49 |
| 75 | Structural and Dynamical Properties of Clusters on A Substrate. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1987, , 241-251. | 0.2 | 0 |
| 76 | Molecular-dynamics simulation of silicon clusters. Physical Review B, 1986, 34, 3910-3916. | 1.1 | 110 |
| 77 | Effect of three-body interactions on the early stages of atomic cluster growth. Chemical Physics Letters, 1986, 124, 84-89. | 1.2 | 17 |
| 78 | 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 |
| 79 | 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 |
| 80 | Effects of three-body interactions on the structure of clusters. Surface Science, 1985, 156, 548-555. | 0.8 | 27 |
| 81 | Electronic structure and vibrational analysis of the alkali peroxides K2O2 and Rb2O2. Chemical Physics Letters, 1984, 108, 237-240. | 1.2 | 5 |
| 82 | Study of the correlated walks with reflecting walls. Journal of Chemical Physics, 1982, 76, 601-608. | 1.2 | 7 |
| 83 | A correlated walk model for thermally stimulated depolarization currents in Î±â€keratin. Journal of Chemical Physics, 1982, 76, 5643-5645. | 1.2 | 4 |
| 84 | 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 |
| 85 | Helixâ€“coil transition of polypeptides on the basis of correlated walks. Journal of Chemical Physics, 1981, 75, 3097-3102. | 1.2 | 14 |
| 86 | The helix-coil transition based on correlated walks. Ferroelectrics, 1980, 30, 299-304. | 0.3 | 2 |
| 87 | 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 |
| 88 | Study of a Lorentzâ€gas based on correlated walks. Journal of Chemical Physics, 1980, 73, 4569-4576. | 1.2 | 16 |
| 89 | 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 |
| 90 | Non-additive interactions in liquid helium solvent effects. Molecular Physics, 1979, 37, 599-606. | 0.8 | 14 |

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| 91 | 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 |
| 92 | Theoretical study on a reaction pathway of Zieglerâ€“Nattaâ€type catalysis. Journal of Chemical Physics, 1978, 68, 2337-2351. | 1.2 | 118 |
| 93 | Role of threeâ€body interactions in trimer binding. Journal of Chemical Physics, 1977, 67, 4701-4705. | 1.2 | 15 |
| 94 | 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 |
| 95 | 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 |
| 96 | 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 |
| 97 | Solvent effects of liquid helium on He2. Molecular Physics, 1976, 31, 1941-1944. | 0.8 | 6 |
| 98 | 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 |
| 99 | Calculation of the Magnetic Moment of Atomic Oxygen. Physical Review, 1969, 177, 432-434. | 2.7 | 8 |
| 100 | Calculation of the Magnetic Moment of Atomic Fluorine. Physical Review, 1968, 172, 44-49. | 2.7 | 11 |