Erik E Santiso

List of Publications by Year
in descending order

67	1,596	293460 24	371746 37
papers	citations	h-index	g-index

68	68	68	2417
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Multiscale Constitutive Modeling of the Mechanical Properties of Polypropylene Fibers from Molecular Simulation Data. Macromolecules, 2022, 55, 728-744.	2.2	5
2	Current Advances in Characterization of Nano-porous Materials: Pore Size Distribution and Surface Area. Engineering Materials, 2021, , 315-340.	0.3	10
3	Can we define a unique microscopic pressure in inhomogeneous fluids?. Journal of Chemical Physics, 2021, 154, 084502.	1.2	12
4	SAFT-Î³-Mie Cross-Interaction Parameters from Density Functional Theory-Predicted Multipoles of Molecular Fragments for Carbon Dioxide, Benzene, Alkanes, and Water. Journal of Physical Chemistry B, 2021, 125, 3867-3882.	1.2	3
5	DFT Analysis of Organotin Catalytic Mechanisms in Dehydration Esterification Reactions for Terephthalic Acid and 2,2,4,4-Tetramethyl-1,3-cyclobutanediol. Journal of Physical Chemistry A, 2021, 125, 4943-4956.	1.1	0
6	Exploring the physicochemical and morphological properties of peptideâ€hybridized dendrimers (<scp>DendriPeps</scp>) and their aggregates. Journal of Polymer Science, 2020, 58, 2234-2247.	2.0	2
7	The Youngâ€“Laplace equation for a solidâ€“liquid interface. Journal of Chemical Physics, 2020, 153, 191102.	1.2	35
8	Microscopic Pressure Tensor in Cylindrical Geometry: Pressure of Water in a Carbon Nanotube. Journal of Chemical Theory and Computation, 2020, 16, 5548-5561.	2.3	14
9	Effect of Poly(vinyl butyral) Comonomer Sequence on Adhesion to Amorphous Silica: A Coarse-Grained Molecular Dynamics Study. ACS Applied Materials & Interfaces, 2020, 12, 47879-47890.	4.0	10
10	Highly Efficient 1-Octene Hydroformylation at Low Syngas Pressure: From Single-Droplet Screening to Continuous Flow Synthesis. ACS Catalysis, 2020, 10, 7535-7542.	5.5	26
11	Modified gaphene oxide (GO) particles in peptide hydrogels: a hybrid system enabling scheduled delivery of synergistic combinations of chemotherapeutics. Journal of Materials Chemistry B, 2020, 8, 3852-3868.	2.9	22
12	Molecular Simulations of Thermoset Polymers Implementing Theoretical Kinetics with Top-Down Coarse-Grained Models. Macromolecules, 2020, 53, 2310-2322.	2.2	10
13	Understanding and Controlling Food Protein Structure and Function in Foods: Perspectives from Experiments and Computer Simulations. Annual Review of Food Science and Technology, 2020, 11, 365-387.	5.1	33
14	Extending the fused-sphere SAFT-Î³ Mie force field parameterization approach to poly(vinyl butyral) copolymers. Journal of Chemical Physics, 2020, 152, 044903.	1.2	6
15	Conformal Sites Theory for Adsorbed Films on Energetically Heterogeneous Surfaces. Langmuir, 2020, 36, 1822-1838.	1.6	7
16	Molecular simulation of polymers with a SAFT-Î³ Mie approach. Molecular Simulation, 2019, 45, 1223-1241.	0.9	10
17	Molecular Modeling Applications in Crystallization. , 2019, , 136-171.		3
18	Understanding Polymorph Selection of Sulfamerazine in Solution. Crystal Growth and Design, 2019, 19, 6925-6934.	1.4	8

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19	Thermomechanical and Free-Volume Properties of Polyesterâ€“Polyol Films for Coatings Applications: Role of Diol Composition. ACS Applied Polymer Materials, 2019, 1, 2398-2406.	2.0	2
20	Morphology and proton diffusion in a coarse-grained model of sulfonated poly(phenylenes). Journal of Chemical Physics, 2019, 151, 104901.	1.2	18
21	Development of a fused-sphere SAFT-Î³ Mie force field for poly(vinyl alcohol) and poly(ethylene). Journal of Chemical Physics, 2019, 150, 034901.	1.2	15
22	A CGenFFâ€based force field for simulations of peptoids with both cis and trans peptide bonds. Journal of Computational Chemistry, 2019, 40, 1946-1956.	1.5	29
23	Bottom-Up Approach to the Coarse-Grained Surface Model: Effective Solidâ€“Fluid Potentials for Adsorption on Heterogeneous Surfaces. Langmuir, 2019, 35, 5975-5986.	1.6	17
24	Oxygen Vacancy Creation Energy in Mn-Containing Perovskites: An Effective Indicator for Chemical Looping with Oxygen Uncoupling. Chemistry of Materials, 2019, 31, 689-698.	3.2	41
25	Spectroscopic and Rheological Cross-Analysis of Polyester Polyol Cure Behavior: Role of Polyester Secondary Hydroxyl Content. ACS Omega, 2019, 4, 932-939.	1.6	11
26	The Nitric Oxide Dimer Reaction in Carbon Nanopores. Journal of Physical Chemistry B, 2018, 122, 3604-3614.	1.2	17
27	Modeling Polymer Glass Transition Properties from Empirical Monomer Data with the SAFT-Î³ Mie Force Field. Macromolecules, 2018, 51, 9526-9537.	2.2	16
28	Ab initio analysis of nucleation reactions during tungsten atomic layer deposition on Si(100) and W(110) substrates. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2018, 36, 061507.	0.9	4
29	Carbon Sequestration through CO2 Foam-Enhanced Oil Recovery: A Green Chemistry Perspective. Engineering, 2018, 4, 336-342.	3.2	51
30	Surface-Driven High-Pressure Processing. Engineering, 2018, 4, 311-320.	3.2	11
31	High-density equation of state for a two-dimensional Lennard-Jones solid. Journal of Chemical Physics, 2018, 148, 174505.	1.2	9
32	Modelling nucleation from solution with the string method in the osmotic ensemble. Molecular Physics, 2018, 116, 2998-3007.	0.8	16
33	Pressure Enhancement in Confined Fluids: Effect of Molecular Shape and Fluidâ€“Wall Interactions. Langmuir, 2017, 33, 11231-11245.	1.6	30
34	Computationally Mapping pK_a Shifts Due to the Presence of a Polyelectrolyte Chain around Whey Proteins. Langmuir, 2017, 33, 11417-11428.	1.6	32
35	Molecular modeling studies of peptoid polymers. AIMS Materials Science, 2017, 4, 1029-1051.	0.7	19
36	Heterogeneous nucleation from a supercooled ionic liquid on a carbon surface. Journal of Chemical Physics, 2016, 145, 211919.	1.2	11

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37	A combined approach for predicting the cytotoxic effect of drug-nanoaggregates. Journal of Materials Chemistry B, 2016, 4, 6516-6523.	2.9	5
38	Perovskite-structured AMn_xB_{1â^'x}O₃ (A = Ca or Ba; B = Fe or Ni) redox catalysts for partial oxidation of methane. Catalysis Science and Technology, 2016, 6, 4535-4544.	2.1	54
39	Homogeneous Nucleation of [dmim+][Clâ^'] from its Supercooled Liquid Phase: A Molecular Simulation Study. Molecular Modeling and Simulation, 2016, , 107-123.	0.2	0
40	Molecular simulation of homogeneous nucleation of crystals of an ionic liquid from the melt. Journal of Chemical Physics, 2015, 143, 124506.	1.2	11
41	A general method for molecular modeling of nucleation from the melt. Journal of Chemical Physics, 2015, 143, 174109.	1.2	19
42	On the connection between nonmonotonic taste behavior and molecular conformation in solution: The case of rebaudioside-A. Journal of Chemical Physics, 2015, 143, 244301.	1.2	10
43	Modelling the interfacial behaviour of dilute light-switching surfactant solutions. Journal of Colloid and Interface Science, 2015, 445, 16-23.	5.0	36
44	Solvent and additive interactions as determinants in the nucleation pathway: general discussion. Faraday Discussions, 2015, 179, 383-420.	1.6	18
45	Understanding the effect of adsorption on activated processes using molecular theory and simulation. Molecular Simulation, 2014, 40, 664-677.	0.9	2
46	Design of Linear Ligands for Selective Separation Using a Genetic Algorithm Applied to Molecular Architecture. Journal of Chemical Information and Modeling, 2013, 53, 1638-1660.	2.5	4
47	On the Calculation of Solid-Fluid Contact Angles from Molecular Dynamics. Entropy, 2013, 15, 3734-3745.	1.1	66
48	Computer Simulations of Homogeneous Nucleation of Benzene from the Melt. Journal of Physical Chemistry B, 2011, 115, 10400-10412.	1.2	37
49	Binding Affinity of a Small Molecule to an Amorphous Polymer in a Solvent. Part 2: Preferential Binding to Local Sites on a Surface. Langmuir, 2011, 27, 12396-12404.	1.6	5
50	A general set of order parameters for molecular crystals. Journal of Chemical Physics, 2011, 134, 064109.	1.2	87
51	Separation of Chemical Reaction Intermediates by Metalâ€“Organic Frameworks. Small, 2011, 7, 2356-2364.	5.2	48
52	Sequestration and selective oxidation of carbon monoxide on graphene edges. Journal of Physics Condensed Matter, 2009, 21, 355008.	0.7	5
53	Isomerization kinetics of small hydrocarbons in confinement. Adsorption, 2008, 14, 181-188.	1.4	5
54	Catalytic role of carbons in methane decomposition for CO- and CO2-free hydrogen generation. Journal of Chemical Physics, 2008, 128, 214702.	1.2	34

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55	A remarkable shape-catalytic effect of confinement on the rotational isomerization of small hydrocarbons. Journal of Chemical Physics, 2008, 128, 034704.	1.2	25
56	Theoretical study of kinetics of zipping phenomena in biomimetic polymers. Physical Review E, 2007, 76, 011915.	0.8	1
57	Confinement effects on chemical reactionsâ€"Toward an integrated rational catalyst design. Applied Surface Science, 2007, 253, 5570-5579.	3.1	40
58	An efficient and robust algorithm for the calculation of gasâ€"liquid critical point of multicomponent petroleum fluids. Fluid Phase Equilibria, 2006, 241, 186-195.	1.4	22
59	Curvature dependency of surface tension in multicomponent systems. AICHE Journal, 2006, 52, 311-322.	1.8	32
60	Effect of confinement by porous carbons on the unimolecular decomposition of formaldehyde. Journal of Chemical Physics, 2006, 125, 084711.	1.2	17
61	Adsorption and catalysis: The effect of confinement on chemical reactions. Applied Surface Science, 2005, 252, 766-777.	3.1	85
62	Effect of Confinement on Chemical Reactions. Adsorption, 2005, 11, 349-354.	1.4	28
63	Effect of Confinement on Freezing of CCl4 in Cylindrical Pores. Adsorption, 2005, 11, 391-396.	1.4	17
64	Molecular modeling of freezing of simple fluids confined within carbon nanotubes. Journal of Chemical Physics, 2005, 122, 144706.	1.2	48
65	Dissociation of Water on Defective Carbon Substrates. Physical Review Letters, 2005, 95, 136105.	2.9	139
66	Multi-scale Molecular Modeling of Chemical Reactivity. Molecular Simulation, 2004, 30, 699-748.	0.9	60
67	Dense packing of binary and polydisperse hard spheres. Molecular Physics, 2002, 100, 2461-2469.	0.8	71