Gerassimos Orkoulas

List of Publications by Year
in descending order

55 papers	**1,761** citations	257450 **24** h-index	265206 **42** g-index
56 all docs	**56** docs citations	**56** times ranked	**1488** citing authors

#	Article	IF	Citations
1	Phase behavior of the restricted primitive model and square-well fluids from Monte Carlo simulations in the grand canonical ensemble. Journal of Chemical Physics, 1999, 110, 1581-1590.	3.0	231
2	Free energy and phase equilibria for the restricted primitive model of ionic fluids from Monte Carlo simulations. Journal of Chemical Physics, 1994, 101, 1452-1459.	3.0	203
3	Postextraction Separation, On-Board Storage, and Catalytic Conversion of Methane in Natural Gas: A Review. Chemical Reviews, 2016, 116, 11436-11499.	47.7	176
4	CO_2 capture in lignin-derived and nitrogen-doped hierarchical porous carbons. Carbon, 2017, 121, 257-266.	10.3	119
5	Crystal shape and size control using a plug flow crystallization configuration. Chemical Engineering Science, 2014, 119, 30-39.	3.8	86
6	Modeling and control of crystal shape in continuous protein crystallization. Chemical Engineering Science, 2014, 107, 47-57.	3.8	86
7	Modeling and control of protein crystal shape and size in batch crystallization. AICHE Journal, 2013, 59, 2317-2327.	3.6	66
8	Adsorptive separation of CO_2 in sulfur-doped nanoporous carbons: Selectivity and breakthrough simulation. Microporous and Mesoporous Materials, 2017, 241, 226-237.	4.4	53
9	Regulation of film thickness, surface roughness and porosity in thin film growth using deposition rate. Chemical Engineering Science, 2009, 64, 3903-3913.	3.8	42
10	Nanoporous Boron Nitride as Exceptionally Thermally Stable Adsorbent: Role in Efficient Separation of Light Hydrocarbons. ACS Applied Materials & Interfaces, 2017, 9, 14506-14517.	8.0	41
11	Separation of ethane-ethylene and propane-propylene by Ag(I) doped and sulfurized microporous carbon. Microporous and Mesoporous Materials, 2020, 299, 110099.	4.4	40
12	Phase diagram of the two€dimensional Coulomb gas: A thermodynamic scaling Monte Carlo study. Journal of Chemical Physics, 1996, 104, 7205-7209.	3.0	37
13	Modeling and control of film porosity in thin film deposition. Chemical Engineering Science, 2009, 64, 3668-3682.	3.8	37
14	Crystal shape modeling and control in protein crystal growth. Chemical Engineering Science, 2013, 87, 216-223.	3.8	37
15	A method for handling batch-to-batch parametric drift using moving horizon estimation: Application to run-to-run MPC of batch crystallization. Chemical Engineering Science, 2015, 127, 210-219.	3.8	37
16	Machine learning-based modeling and operation for ALD of SiO_2 thin-films using data from a multiscale CFD simulation. Chemical Engineering Research and Design, 2019, 151, 131-145.	5.6	36
17	Modeling and control of shape distribution of protein crystal aggregates. Chemical Engineering Science, 2013, 104, 484-497.	3.8	34
18	Run-to-Run-Based Model Predictive Control of Protein Crystal Shape in Batch Crystallization. Industrial & Engineering Chemistry Research, 2015, 54, 4293-4302.	3.7	34

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19	Protein Crystal Shape and Size Control in Batch Crystallization: Comparing Model Predictive Control with Conventional Operating Policies. Industrial & Engineering Chemistry Research, 2014, 53, 5002-5014.	3.7	33
20	Investigation of film surface roughness and porosity dependence on lattice size in a porous thin film deposition process. Physical Review E, 2009, 80, 041122.	2.1	32
21	Enhancing the Crystal Production Rate and Reducing Polydispersity in Continuous Protein Crystallization. Industrial & Engineering Chemistry Research, 2014, 53, 15538-15548.	3.7	32
22	Modeling and control of ibuprofen crystal growth and size distribution. Chemical Engineering Science, 2015, 134, 414-422.	3.8	32
23	One-step conversion of agro-wastes to nanoporous carbons: Role in separation of greenhouse gases. Bioresource Technology, 2018, 256, 232-240.	9.6	26
24	Stochastic Modeling and Simultaneous Regulation of Surface Roughness and Porosity in Thin Film Deposition. Industrial & Engineering Chemistry Research, 2009, 48, 6690-6700.	3.7	25
25	Synthesis of Nitrogen and Sulfur Codoped Nanoporous Carbons from Algae: Role in CO_2 Separation. ACS Omega, 2018, 3, 18592-18602.	3.5	23
26	Dependence of film surface roughness and slope on surface migration and lattice size in thin film deposition processes. Chemical Engineering Science, 2010, 65, 6101-6111.	3.8	19
27	Dynamics and Lattice-Size Dependence of Surface Mean Slope in Thin-Film Deposition. Industrial & Engineering Chemistry Research, 2011, 50, 1219-1230.	3.7	17
28	Microscopic modeling and optimal operation of plasma enhanced atomic layer deposition. Chemical Engineering Research and Design, 2020, 159, 439-454.	5.6	14
29	Microscopic and data-driven modeling and operation of thermal atomic layer etching of aluminum oxide thin films. Chemical Engineering Research and Design, 2022, 177, 96-107.	5.6	13
30	Multiscale computational fluid dynamics modeling of thermal atomic layer etching: Application to chamber configuration design. Computers and Chemical Engineering, 2022, 161, 107757.	3.8	13
31	Predictive control of surface mean slope and roughness in a thin film deposition process. Chemical Engineering Science, 2010, 65, 4720-4731.	3.8	11
32	Controller and Estimator Design for Regulation of Film Thickness, Surface Roughness, and Porosity in a Multiscale Thin Film Growth Process. Industrial & Engineering Chemistry Research, 2010, 49, 7795-7806.	3.7	10
33	Dynamics and control of aggregate thin film surface morphology for improved light trapping: Implementation on a large-lattice kinetic Monte Carlo model. Chemical Engineering Science, 2011, 66, 5955-5967.	3.8	9
34	Multiscale computational fluid dynamics modeling of spatial thermal atomic layer etching. Computers and Chemical Engineering, 2022, 163, 107861.	3.8	9
35	Modeling and control of Transparent Conducting Oxide layer surface morphology for improved light trapping. Chemical Engineering Science, 2012, 74, 135-147.	3.8	8
36	Surface morphology control of Transparent Conducting Oxide layers for improved light trapping using wafer grating and feedback control. Chemical Engineering Science, 2012, 81, 191-201.	3.8	7

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37	Multivariable run-to-run control of thermal atomic layer etching of aluminum oxide thin films. Chemical Engineering Research and Design, 2022, 182, 1-12.	5.6	7
38	Simulation and control of aggregate surface morphology in a two-stage thin film deposition process for improved light trapping. Chemical Engineering Science, 2012, 71, 520-530.	3.8	6
39	Porosity control in thin film solar cells. Chemical Engineering Science, 2013, 94, 44-53.	3.8	5
40	Multivariable Model Predictive Control of Thin Film Surface Roughness and Slope for Light Trapping Optimization. Industrial & Engineering Chemistry Research, 2010, 49, 10510-10516.	3.7	4
41	Controlling aggregate thin film surface morphology for improved light trapping using a patterned deposition rate profile. Chemical Engineering Science, 2012, 67, 101-110.	3.8	4
42	Simulation and Control of Porosity in a Three-Dimensional Thin-Film Solar Cell. Industrial & Engineering Chemistry Research, 2013, 52, 11246-11252.	3.7	3
43	Stochastic modeling of film porosity in thin film deposition. , 2009, , .		1
44	Computer Simulations: An Overview of Monte Carlo Methods for Fluid Simulation. Computing in Science and Engineering, 2009, 11, 76-87.	1.2	1
45	Modeling and control of aggregate thin film surface morphology using stochastic PDEs and a patterned deposition rate profile. , 2011, , .		1
46	Model predictive control of film porosity in thin film deposition. , 2009, , .		0
47	Simultaneous regulation of film thickness, surface roughness and porosity in a multiscale thin film growth process. , 2009, , .		0
48	Simultaneous Regulation of Surface Roughness and Porosity in Thin Film Growth. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2009, 42, 922-927.	0.4	0
49	Lattice-size Dependence and Dynamics of Surface Mean Slope in a Thin Film Deposition Process. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2010, 43, 811-816.	0.4	0
50	Simultaneous regulation of thin film surface mean slope and roughness for light trapping optimization using predictive control. , 2010, , .		0
51	Multivariable model predictive control of thin film surface roughness and slope: Application to a 2D kinetic Monte-Carlo model. , 2011, , .		0
52	Dependence of film surface roughness on surface migration and lattice size in thin film deposition. , 2011, , .		0
53	Predictive control of aggregate surface morphology in a two-stage thin film deposition process for improved light trapping. , 2012, , .		0
54	Modeling and control of protein crystal shape distribution. , 2013, , .		0

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55	Porosity control in thin film solar cells: Two-dimensional case. , 2013, , .		0