

James W Evans

List of Publications by Year in descending order

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99
papers

1,366
citations

430442

18
h-index

433756

31
g-index

100
all docs

100
docs citations

100
times ranked

1396
citing authors

#	ARTICLE	IF	CITATIONS
1	Growth morphology and properties of metals on graphene. <i>Progress in Surface Science</i> , 2015, 90, 397-443.	3.8	123
2	Mild and Selective Hydrogenation of Nitrate to Ammonia in the Absence of Noble Metals. <i>ACS Catalysis</i> , 2020, 10, 3618-3628.	5.5	83
3	Surface energies, adhesion energies, and exfoliation energies relevant to copper-graphene and copper-graphite systems. <i>Surface Science</i> , 2019, 685, 48-58.	0.8	74
4	Realistic multisite lattice-gas modeling and KMC simulation of catalytic surface reactions: Kinetics and multiscale spatial behavior for CO-oxidation on metal (100) surfaces. <i>Progress in Surface Science</i> , 2013, 88, 393-521.	3.8	61
5	Transition metals on the (0 0 0 1) surface of graphite: Fundamental aspects of adsorption, diffusion, and morphology. <i>Progress in Surface Science</i> , 2014, 89, 219-238.	3.8	60
6	Reshaping, Intermixing, and Coarsening for Metallic Nanocrystals: Nonequilibrium Statistical Mechanical and Coarse-Grained Modeling. <i>Chemical Reviews</i> , 2019, 119, 6670-6768.	23.0	50
7	Adsorbate-enhanced transport of metals on metal surfaces: Oxygen and sulfur on coinage metals. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2010, 28, 1285-1298.	0.9	47
8	Kinetic Monte Carlo Simulation of Statistical Mechanical Models and Coarse-Grained Mesoscale Descriptions of Catalytic Reactionâ€”Diffusion Processes: 1D Nanoporous and 2D Surface Systems. <i>Chemical Reviews</i> , 2015, 115, 5979-6050.	23.0	37
9	Directed assembly of Ru nanoclusters on Ru(0001)-supported graphene: STM studies and atomistic modeling. <i>Physical Review B</i> , 2012, 86, .	1.1	27
10	Formation of Multilayer Cu Islands Embedded beneath the Surface of Graphite: Characterization and Fundamental Insights. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4454-4469.	1.5	27
11	Real-Time Ab Initio KMC Simulation of the Self-Assembly and Sintering of Bimetallic Epitaxial Nanoclusters: Au + Ag on Ag(100). <i>Nano Letters</i> , 2014, 14, 4646-4652.	4.5	25
12	Kinetics, energetics, and size dependence of the transformation from Pt to ordered PtSn intermetallic nanoparticles. <i>Nanoscale</i> , 2019, 11, 5336-5345.	2.8	25
13	Ab Initio Thermodynamics and Kinetics for Coalescence of Two-Dimensional Nanoislands and Nanopits on Metal (100) Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21617-21630.	1.5	24
14	Reverse-engineering of graphene on metal surfaces: a case study of embedded ruthenium. <i>Nanotechnology</i> , 2018, 29, 505601.	1.3	22
15	Strainâ€”Enhanced Metallic Intermixing in Shapeâ€”Controlled Multilayered Coreâ€”Shell Nanostructures: Toward Shaped Intermetallics. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 10574-10580.	7.2	22
16	Thermodynamic Preference for Atom Adsorption on versus Intercalation into Multilayer Graphene. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9725-9730.	2.1	21
17	Dissociative adsorption of O ₂ on unreconstructed metal (100) surfaces: Pathways, energetics, and sticking kinetics. <i>Physical Review B</i> , 2014, 89, .	1.1	20
18	Sierpiński Structure and Electronic Topology in Bi Thin Films on InSb(111)B Surfaces. <i>Physical Review Letters</i> , 2021, 126, 176102.	2.9	20

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19	Adsorption, intercalation, diffusion, and adhesion of Cu at the S_2 surface from first-principles calculations. <i>Physical Review Research</i> , 2020, 2, .	1.3	20
20	Nanoscale ϵ -Quantum Islands on Metal Substrates: Microscopy Studies and Electronic Structure Analyses. <i>Materials</i> , 2010, 3, 3965-3993.	1.3	18
21	A Little Chemistry Helps the Big Get Bigger. <i>Science</i> , 2010, 330, 599-600.	6.0	18
22	Interactions between Oxygen Atoms on Pt(100): Implications for Ordering during Chemisorption and Catalysis. <i>ChemPhysChem</i> , 2010, 11, 2174-2181.	1.0	17
23	Predictive Beyond-Mean-Field Rate Equations for Multisite Lattice Gas Models of Catalytic Surface Reactions: CO Oxidation on Pd(100). <i>Journal of Physical Chemistry C</i> , 2016, 120, 28639-28653.	1.5	17
24	Reshaping and sintering of 3D fcc metal nanoclusters: Stochastic atomistic modeling with realistic surface diffusion kinetics. <i>Physical Review Materials</i> , 2019, 3, .	0.9	16
25	Pore diameter dependence of catalytic activity: <i>p</i> -nitrobenzaldehyde conversion to an aldol product in amine-functionalized mesoporous silica. <i>Journal of Chemical Physics</i> , 2018, 149, 024101.	1.2	15
26	Energetics of Cu adsorption and intercalation at graphite step edges. <i>Physical Review B</i> , 2019, 99, .	1.1	15
27	Squeezed nanocrystals: equilibrium configuration of metal clusters embedded beneath the surface of a layered material. <i>Nanoscale</i> , 2019, 11, 6445-6452.	2.8	14
28	Fabricating Fe nanocrystals via encapsulation at the graphite surface. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2019, 37, 061403.	0.9	14
29	Shapes of Fe nanocrystals encapsulated at the graphite surface. <i>New Journal of Physics</i> , 2020, 22, 023016.	1.2	14
30	Interplay between Anomalous Transport and Catalytic Reaction Kinetics in Single-File Nanoporous Systems. <i>ACS Catalysis</i> , 2011, 1, 751-763.	5.5	13
31	Generalized Hydrodynamic Treatment of the Interplay between Restricted Transport and Catalytic Reactions in Nanoporous Materials. <i>Physical Review Letters</i> , 2012, 108, 228301.	2.9	13
32	Point island models for nucleation and growth of supported nanoclusters during surface deposition. <i>Journal of Chemical Physics</i> , 2016, 145, 211904.	1.2	13
33	Thickness-dependent energetics for Pb adatoms on low-index Pb nanofilm surfaces: First-principles calculations. <i>Physical Review B</i> , 2017, 96, .	1.1	13
34	Mechanism of Metal Intercalation under Graphene through Small Vacancy Defects. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6954-6962.	1.5	13
35	Nucleation and growth kinetics for intercalated islands during deposition on layered materials with isolated pointlike surface defects. <i>Physical Review Materials</i> , 2017, 1, .	0.9	13
36	Anisotropic coarsening: One-dimensional decay of Ag islands on Ag(110). <i>Physical Review B</i> , 2013, 87, .	1.1	12

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37	Transitions between strongly correlated and random steady-states for catalytic CO-oxidation on surfaces at high-pressure. <i>Journal of Chemical Physics</i> , 2015, 142, 134703.	1.2	12
38	Kinetics of the functionalization of mesoporous silica nanoparticles: Implications on surface group distributions, adsorption and catalysis. <i>Microporous and Mesoporous Materials</i> , 2020, 305, 110276.	2.2	12
39	Dy adsorption on and intercalation under graphene on 6H-SiC(0001) surface from first-principles calculations. <i>Physical Review Materials</i> , 2021, 5, .	0.9	12
40	Non-equilibrium growth of metal clusters on a layered material: Cu on MoS ₂ . <i>New Journal of Physics</i> , 2020, 22, 053033.	1.2	12
41	Catalytic conversion reactions mediated by single-file diffusion in linear nanopores: Hydrodynamic versus stochastic behavior. <i>Journal of Chemical Physics</i> , 2011, 134, 114107.	1.2	10
42	Atomistic modeling of the directed-assembly of bimetallic Pt-Ru nanoclusters on Ru(0001)-supported monolayer graphene. <i>Journal of Chemical Physics</i> , 2013, 138, 134703.	1.2	10
43	Refined BCF-type boundary conditions for mesoscale surface step dynamics. <i>Physical Review B</i> , 2015, 91, .	1.1	10
44	Communication: Diverse nanoscale cluster dynamics: Diffusion of 2D epitaxial clusters. <i>Journal of Chemical Physics</i> , 2017, 147, 201101.	1.2	10
45	Encapsulation of metal nanoparticles at the surface of a prototypical layered material. <i>Nanoscale</i> , 2021, 13, 1485-1506.	2.8	10
46	Diffusion of two-dimensional epitaxial clusters on metal (100) surfaces: Facile versus nucleation-mediated behavior and their merging for larger sizes. <i>Physical Review B</i> , 2017, 96, .	1.1	10
47	Adsorption of dysprosium on the graphite (0001) surface: Nucleation and growth at 300 K. <i>Journal of Chemical Physics</i> , 2016, 145, 211902.	1.2	9
48	Size Dependence of S-bonding on (111) Facets of Cu Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10268-10274.	1.5	9
49	Reshaping of Truncated Pd Nanocubes: Energetic and Kinetic Analysis Integrating Transmission Electron Microscopy with Atomistic-Level and Coarse-Grained Modeling. <i>ACS Nano</i> , 2020, 14, 8551-8561.	7.3	9
50	Statistical mechanical models for dissociative adsorption of O ₂ on metal(100) surfaces with blocking, steering, and funneling. <i>Journal of Chemical Physics</i> , 2014, 140, 194704.	1.2	8
51	Adsorption and diffusion of Ru adatoms on Ru(0001)-supported graphene: Large-scale first-principles calculations. <i>Journal of Chemical Physics</i> , 2015, 143, 164706.	1.2	8
52	Fundamentals of Au(111) Surface Dynamics: Coarsening of Two-Dimensional Au Islands. <i>Journal of Physical Chemistry C</i> , 2020, 124, 7492-7499.	1.5	8
53	Energy barriers for Dy and H penetrating graphene on 6H-SiC(0001) and freestanding bilayer graphene from first-principles calculations. <i>Applied Physics Letters</i> , 2021, 119, .	1.5	8
54	Thermodynamics and kinetics of H adsorption and intercalation for graphene on 6H-SiC(0001) from first-principles calculations. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2022, 40, .	0.9	8

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55	Directing Anisotropic Assembly of Metallic Nanoclusters by Exploiting Linear Trio Interactions and Quantum Size Effects: Au Chains on Ag(100) Thin Films. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2194-2199.	2.1	7
56	Structure of Polydisperse fcc Nanocrystals: Implications for Crystal Fractionalization. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9528-9537.	1.5	7
57	Controlling reactivity of nanoporous catalyst materials by tuning reaction product-pore interior interactions: Statistical mechanical modeling. <i>Journal of Chemical Physics</i> , 2013, 138, 134705.	1.2	6
58	Langevin and Fokker-Planck Analyses of Inhibited Molecular Passing Processes Controlling Transport and Reactivity in Nanoporous Materials. <i>Physical Review Letters</i> , 2014, 113, 038301.	2.9	6
59	Discontinuous non-equilibrium phase transition in a threshold Schloegl model for autocatalysis: Generic two-phase coexistence and metastability. <i>Journal of Chemical Physics</i> , 2015, 142, 164105.	1.2	6
60	Comparison of S-adsorption on (111) and (100) facets of Cu nanoclusters. <i>Journal of Chemical Physics</i> , 2016, 145, 164312.	1.2	6
61	Capture zone area distributions for nucleation and growth of islands during submonolayer deposition. <i>Journal of Chemical Physics</i> , 2016, 145, 211911.	1.2	6
62	Stability of M ₃ S ₃ complexes on fcc M(111) surfaces: M = Au, Ag, Cu, and Ni. <i>Surface Science</i> , 2018, 676, 2-8.	0.8	6
63	Competitive formation of intercalated versus supported metal nanoclusters during deposition on layered materials with surface point defects. <i>Journal of Chemical Physics</i> , 2021, 154, 024703.	1.2	6
64	Reaction processes at step edges on S-decorated Cu(111) and Ag(111) surfaces: MD analysis utilizing machine learning derived potentials. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	6
65	Permeability and kinetic coefficients for mesoscale BCF surface step dynamics: Discrete two-dimensional deposition-diffusion equation analysis. <i>Physical Review B</i> , 2016, 93, .	1.1	5
66	Coinage Metal-Sulfur Complexes: Stability on Metal(111) Surfaces and in the Gas Phase. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12954-12965.	1.5	5
67	Sulfur adsorption on coinage metal(100) surfaces: propensity for metal-sulfur complex formation relative to (111) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26483-26491.	1.3	5
68	Structure of chalcogen overlayers on Au(111): Density functional theory and lattice-gas modeling. <i>Journal of Chemical Physics</i> , 2020, 152, 224706.	1.2	5
69	Effective Fragment Potential-Based Molecular Dynamics Studies of Diffusion in Acetone and Hexane. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3398-3405.	1.1	5
70	Thermodynamically Driven Formation of Intercalated Cu Carpets from Supported Cu Pyramids on MoS ₂ . <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6651-6656.	2.1	5
71	Adsorption and Diffusion of Gallium Adatoms on the Si(100)-2 × 1 Reconstructed Surface: A Multiconfiguration Self-Consistent Field Study Utilizing Molecular Surface Clusters. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23488-23500.	1.5	4
72	Analytic formulations for one-dimensional decay of rectangular homoepitaxial islands during coarsening on anisotropic fcc (110) surfaces. <i>Physical Review B</i> , 2013, 88, .	1.1	4

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73	Submonolayer Ag films on Fe(100): A first-principles analysis of energetics controlling adlayer thermodynamics and kinetics. <i>Physical Review B</i> , 2016, 93, .	1.1	4
74	Tailoring Kinetics on a Topological Insulator Surface by Defect-Induced Strain: Pb Mobility on Bi_2Te_3 . <i>Nano Letters</i> , 2016, 16, 4454-4461.	4.5	4
75	Discontinuous Phase Transitions in Nonlocal Schloegl Models for Autocatalysis: Loss and Reemergence of a Nonequilibrium Gibbs Phase Rule. <i>Physical Review Letters</i> , 2018, 121, 120603.	2.9	4
76	Energy barriers for Pb adatom diffusion on stepped ultrathin Pb(111) quantum nanofilms: First-principles calculations. <i>Physical Review B</i> , 2019, 100, .	1.1	4
77	Surface structure of linear nanopores in amorphous silica: Comparison of properties for different pore generation algorithms. <i>Journal of Chemical Physics</i> , 2020, 153, 124708.	1.2	4
78	Tricriticality in generalized Schloegl models for autocatalysis: Lattice-gas realization with particle diffusion. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2012, 391, 633-646.	1.2	3
79	Modeling of Diffusivity for 2D Vacancy Nanopits and Comparison with 2D Adatom Nanoislands on Metal(100) Surfaces Including Analysis for Ag(100). <i>Journal of Physical Chemistry C</i> , 2018, 122, 11334-11344.	1.5	3
80	Complex oscillatory decrease with size in diffusivity of {100}-epitaxially supported 3D fcc metal nanoclusters. <i>Nanoscale</i> , 2019, 11, 17506-17516.	2.8	3
81	Extended families of critical and stationary droplets for nonequilibrium phase transitions in spatially discrete bistable systems. <i>Physical Review E</i> , 2020, 101, 022803.	0.8	3
82	Enhanced Nanostructure Dynamics on Au(111) with Adsorbed Sulfur due to Au^+S Complex Formation. <i>ChemPhysChem</i> , 2021, 22, 349-358.	1.0	3
83	Molecular interactions in diffusion-controlled aldol condensation with mesoporous silica nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 10475-10487.	1.3	3
84	Catalytic conversion in nanoporous materials: Concentration oscillations and spatial correlations due to inhibited transport and intermolecular interactions. <i>Journal of Chemical Physics</i> , 2016, 145, 174705.	1.2	2
85	Catalytic conversion reactions in nanoporous systems with concentration-dependent selectivity: Statistical mechanical modeling. <i>Physical Review E</i> , 2016, 93, 052137.	0.8	2
86	Tracer counterpermeation analysis of diffusivity in finite-length nanopores with and without single-file dynamics. <i>Physical Review E</i> , 2017, 95, 012132.	0.8	2
87	Strain-Enhanced Metallic Intermixing in Shape-Controlled Multilayered Core-Shell Nanostructures: Toward Shaped Intermetallics. <i>Angewandte Chemie</i> , 2020, 132, 10661-10667.	1.6	2
88	Shape Stability of Truncated Octahedral fcc Metal Nanocrystals. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 51954-51961.	4.0	2
89	Equilibrium shapes of faceted 3D metal nanoclusters intercalated near the surface of layered materials. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 445001.	0.7	2
90	Boundary Conditions for Diffusion-Mediated Processes within Linear Nanopores: Exact Treatment of Coupling to an Equilibrated External Fluid. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8873-8888.	1.5	1

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91	Generalized hydrodynamic analysis of transport through a finite open nanopore for two-component single-file systems. <i>Physical Review E</i> , 2020, 101, 062103.	0.8	1
92	Phase transitions in Schloegl's second model for autocatalysis on a Bethe lattice. <i>Physical Review E</i> , 2021, 104, 014135.	0.8	1
93	Sulfur-enhanced dynamics of coinage metal(111) surfaces: Step edges versus terraces as locations for metal-sulfur complex formation. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2022, 40, 023205.	0.9	1
94	Rotational and translational diffusion of liquid n-hexane: EFP-based molecular dynamics analysis. <i>Journal of Chemical Physics</i> , 2022, 156, 114503.	1.2	1
95	Atomistic and Coarse-Grained Modeling Strategies for Thin Film Nucleation and Growth on Quasicrystalline Surfaces. <i>Materials Research Society Symposia Proceedings</i> , 2013, 1517, 1.	0.1	0
96	Enhanced Nanostructure Dynamics on Au(111) with Adsorbed Sulfur due to Au ⁺ S Complex Formation. <i>ChemPhysChem</i> , 2021, 22, 343-343.	1.0	0
97	Anomalous Kinetics of Catalytic Conversion Reactions in Linear Nanopores Mediated by Inhibited Transport: Multiscale Modeling. , 2019, , 173-190.		0
98	Preface for the special collection commemorating the career of Pat Thiel. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2022, 40, 031601.	0.9	0
99	Modeling of linear nanopores in α -SiO ₂ tuning pore surface structure. <i>Microporous and Mesoporous Materials</i> , 2022, , 112077.	2.2	0