James W Evans

List of Publications by Year
in descending order

99 papers	1,366 citations	430874 18 h-index	434195 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. Progress in Surface Science, 2015, 90, 397-443.	8.3	123
2	Mild and Selective Hydrogenation of Nitrate to Ammonia in the Absence of Noble Metals. ACS Catalysis, 2020, 10, 3618-3628.	11.2	83
3	Surface energies, adhesion energies, and exfoliation energies relevant to copper-graphene and copper-graphite systems. Surface Science, 2019, 685, 48-58.	1.9	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. Progress in Surface Science, 2013, 88, 393-521.	8.3	61
5	Transition metals on the (0 0 0 1) surface of graphite: Fundamental aspects of adsorption, diffusion, and morphology. Progress in Surface Science, 2014, 89, 219-238.	8.3	60
6	Reshaping, Intermixing, and Coarsening for Metallic Nanocrystals: Nonequilibrium Statistical Mechanical and Coarse-Grained Modeling. Chemical Reviews, 2019, 119, 6670-6768.	47.7	50
7	Adsorbate-enhanced transport of metals on metal surfaces: Oxygen and sulfur on coinage metals. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2010, 28, 1285-1298.	2.1	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. Chemical Reviews, 2015, 115, 5979-6050.	47.7	37
9	Directed assembly of Ru nanoclusters on Ru(0001)-supported graphene: STM studies and atomistic modeling. Physical Review B, 2012, 86, .	3.2	27
10	Formation of Multilayer Cu Islands Embedded beneath the Surface of Graphite: Characterization and Fundamental Insights. Journal of Physical Chemistry C, 2018, 122, 4454-4469.	3.1	27
11	Real-Time Ab Initio KMC Simulation of the Self-Assembly and Sintering of Bimetallic Epitaxial Nanoclusters: Au + Ag on Ag(100). Nano Letters, 2014, 14, 4646-4652.	9.1	25
12	Kinetics, energetics, and size dependence of the transformation from Pt to ordered PtSn intermetallic nanoparticles. Nanoscale, 2019, 11, 5336-5345.	5.6	25
13	Ab Initio Thermodynamics and Kinetics for Coalescence of Two-Dimensional Nanoislands and Nanopits on Metal (100) Surfaces. Journal of Physical Chemistry C, 2016, 120, 21617-21630.	3.1	24
14	Reverse-engineering of graphene on metal surfaces: a case study of embedded ruthenium. Nanotechnology, 2018, 29, 505601.	2.6	22
15	Strainâ€Enhanced Metallic Intermixing in Shapeâ€Controlled Multilayered Coreâ€“Shell Nanostructures: Toward Shaped Intermetallics. Angewandte Chemie - International Edition, 2020, 59, 10574-10580.	13.8	22
16	Thermodynamic Preference for Atom Adsorption on versus Intercalation into Multilayer Graphene. Journal of Physical Chemistry Letters, 2020, 11, 9725-9730.	4.6	21
17	Dissociative adsorption of O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>on unreconstructed metal (100) surfaces: Pathways, energetics, and sticking kinetics. Physical Review B, 2014, 89, .	3.2	20
18	SierpiÅ„ski Structure and Electronic Topology in Bi Thin Films on InSb(111)B Surfaces. Physical Review Letters, 2021, 126, 176102.	7.8	20

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19	Adsorption, intercalation, diffusion, and adhesion of Cu at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> (0001) surface from first-principles calculations. Physical Review Research, 2020, 2, .	3.6	20
20	Nanoscale â€œQuantumâ€•Islands on Metal Substrates: Microscopy Studies and Electronic Structure Analyses. Materials, 2010, 3, 3965-3993.	2.9	18
21	A Little Chemistry Helps the Big Get Bigger. Science, 2010, 330, 599-600.	12.6	18
22	Interactions between Oxygen Atoms on Pt(100): Implications for Ordering during Chemisorption and Catalysis. ChemPhysChem, 2010, 11, 2174-2181.	2.1	17
23	Predictive Beyond-Mean-Field Rate Equations for Multisite Latticeâ€“Gas Models of Catalytic Surface Reactions: CO Oxidation on Pd(100). Journal of Physical Chemistry C, 2016, 120, 28639-28653.	3.1	17
24	Reshaping and sintering of 3D fcc metal nanoclusters: Stochastic atomistic modeling with realistic surface diffusion kinetics. Physical Review Materials, 2019, 3, .	2.4	16
25	Pore diameter dependence of catalytic activity: p-nitrobenzaldehyde conversion to an aldol product in amine-functionalized mesoporous silica. Journal of Chemical Physics, 2018, 149, 024101.	3.0	15
26	Energetics of Cu adsorption and intercalation at graphite step edges. Physical Review B, 2019, 99, .	3.2	15
27	Squeezed nanocrystals: equilibrium configuration of metal clusters embedded beneath the surface of a layered material. Nanoscale, 2019, 11, 6445-6452.	5.6	14
28	Fabricating Fe nanocrystals via encapsulation at the graphite surface. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2019, 37, 061403.	2.1	14
29	Shapes of Fe nanocrystals encapsulated at the graphite surface. New Journal of Physics, 2020, 22, 023016.	2.9	14
30	Interplay between Anomalous Transport and Catalytic Reaction Kinetics in Single-File Nanoporous Systems. ACS Catalysis, 2011, 1, 751-763.	11.2	13
31	Generalized Hydrodynamic Treatment of the Interplay between Restricted Transport and Catalytic Reactions in Nanoporous Materials. Physical Review Letters, 2012, 108, 228301.	7.8	13
32	Point island models for nucleation and growth of supported nanoclusters during surface deposition. Journal of Chemical Physics, 2016, 145, 211904.	3.0	13
33	Thickness-dependent energetics for Pb adatoms on low-index Pb nanofilm surfaces: First-principles calculations. Physical Review B, 2017, 96, .	3.2	13
34	Mechanism of Metal Intercalation under Graphene through Small Vacancy Defects. Journal of Physical Chemistry C, 2021, 125, 6954-6962.	3.1	13
35	Nucleation and growth kinetics for intercalated islands during deposition on layered materials with isolated pointlike surface defects. Physical Review Materials, 2017, 1, .	2.4	13
36	Anisotropic coarsening: One-dimensional decay of Ag islands on Ag(110). Physical Review B, 2013, 87, .	3.2	12

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37	Transitions between strongly correlated and random steady-states for catalytic CO-oxidation on surfaces at high-pressure. Journal of Chemical Physics, 2015, 142, 134703.	3.0	12
38	Kinetics of the functionalization of mesoporous silica nanoparticles: Implications on surface group distributions, adsorption and catalysis. Microporous and Mesoporous Materials, 2020, 305, 110276.	4.4	12
39	Dy adsorption on and intercalation under graphene on 6 H -SiC(0001) surface from first-principles calculations. Physical Review Materials, 2021, 5, .	2.4	12
40	Non-equilibrium growth of metal clusters on a layered material: Cu on MoS₂. New Journal of Physics, 2020, 22, 053033.	2.9	12
41	Catalytic conversion reactions mediated by single-file diffusion in linear nanopores: Hydrodynamic versus stochastic behavior. Journal of Chemical Physics, 2011, 134, 114107.	3.0	10
42	Atomistic modeling of the directed-assembly of bimetallic Pt-Ru nanoclusters on Ru(0001)-supported monolayer graphene. Journal of Chemical Physics, 2013, 138, 134703.	3.0	10
43	Refined BCF-type boundary conditions for mesoscale surface step dynamics. Physical Review B, 2015, 91, .	3.2	10
44	Communication: Diverse nanoscale cluster dynamics: Diffusion of 2D epitaxial clusters. Journal of Chemical Physics, 2017, 147, 201101.	3.0	10
45	Encapsulation of metal nanoparticles at the surface of a prototypical layered material. Nanoscale, 2021, 13, 1485-1506.	5.6	10
46	Diffusion of two-dimensional epitaxial clusters on metal (100) surfaces: Facile versus nucleation-mediated behavior and their merging for larger sizes. Physical Review B, 2017, 96, .	3.2	10
47	Adsorption of dysprosium on the graphite (0001) surface: Nucleation and growth at 300 K. Journal of Chemical Physics, 2016, 145, 211902.	3.0	9
48	Size Dependence of S-bonding on (111) Facets of Cu Nanoclusters. Journal of Physical Chemistry C, 2016, 120, 10268-10274.	3.1	9
49	Reshaping of Truncated Pd Nanocubes: Energetic and Kinetic Analysis Integrating Transmission Electron Microscopy with Atomistic-Level and Coarse-Grained Modeling. ACS Nano, 2020, 14, 8551-8561.	14.6	9
50	Statistical mechanical models for dissociative adsorption of O2on metal(100) surfaces with blocking, steering, and funneling. Journal of Chemical Physics, 2014, 140, 194704.	3.0	8
51	Adsorption and diffusion of Ru adatoms on Ru(0001)-supported graphene: Large-scale first-principles calculations. Journal of Chemical Physics, 2015, 143, 164706.	3.0	8
52	Fundamentals of Au(111) Surface Dynamics: Coarsening of Two-Dimensional Au Islands. Journal of Physical Chemistry C, 2020, 124, 7492-7499.	3.1	8
53	Energy barriers for Dy and H penetrating graphene on 6H-SiC(0001) and freestanding bilayer graphene from first-principles calculations. Applied Physics Letters, 2021, 119, .	3.3	8
54	Thermodynamics and kinetics of H adsorption and intercalation for graphene on 6H-SiC(0001) from first-principles calculations. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2022, 40, .	2.1	8

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55	Directing Anisotropic Assembly of Metallic Nanoclusters by Exploiting Linear Trio Interactions and Quantum Size Effects: AuÂChains on Ag(100) Thin Films. Journal of Physical Chemistry Letters, 2015, 6, 2194-2199.	4.6	7
56	Structure of Polydisperse fcc Nanocrystals: Implications for Crystal Fractionalization. Journal of Physical Chemistry C, 2019, 123, 9528-9537.	3.1	7
57	Controlling reactivity of nanoporous catalyst materials by tuning reaction product-pore interior interactions: Statistical mechanical modeling. Journal of Chemical Physics, 2013, 138, 134705.	3.0	6
58	Langevin and Fokker-Planck Analyses of Inhibited Molecular Passing Processes Controlling Transport and Reactivity in Nanoporous Materials. Physical Review Letters, 2014, 113, 038301.	7.8	6
59	Discontinuous non-equilibrium phase transition in a threshold Schloegl model for autocatalysis: Generic two-phase coexistence and metastability. Journal of Chemical Physics, 2015, 142, 164105.	3.0	6
60	Comparison of S-adsorption on (111) and (100) facets of Cu nanoclusters. Journal of Chemical Physics, 2016, 145, 164312.	3.0	6
61	Capture zone area distributions for nucleation and growth of islands during submonolayer deposition. Journal of Chemical Physics, 2016, 145, 211911.	3.0	6
62	Stability of M3S3 complexes on fcc M(111) surfaces: M = Au, Ag, Cu, and Ni. Surface Science, 2018, 676, 2-8.	1.9	6
63	Competitive formation of intercalated versus supported metal nanoclusters during deposition on layered materials with surface point defects. Journal of Chemical Physics, 2021, 154, 024703.	3.0	6
64	Reaction processes at step edges on S-decorated Cu(111) and Ag(111) surfaces: MD analysis utilizing machine learning derived potentials. Journal of Chemical Physics, 2022, 156, .	3.0	6
65	Permeability and kinetic coefficients for mesoscale BCF surface step dynamics: Discrete two-dimensional deposition-diffusion equation analysis. Physical Review B, 2016, 93, .	3.2	5
66	Coinage Metalâ€“Sulfur Complexes: Stability on Metal(111) Surfaces and in the Gas Phase. Journal of Physical Chemistry C, 2019, 123, 12954-12965.	3.1	5
67	Sulfur adsorption on coinage metal(100) surfaces: propensity for metalâ€“sulfur complex formation relative to (111) surfaces. Physical Chemistry Chemical Physics, 2019, 21, 26483-26491.	2.8	5
68	Structure of chalcogen overlayers on Au(111): Density functional theory and lattice-gas modeling. Journal of Chemical Physics, 2020, 152, 224706.	3.0	5
69	Effective Fragment Potential-Based Molecular Dynamics Studies of Diffusion in Acetone and Hexane. Journal of Physical Chemistry A, 2021, 125, 3398-3405.	2.5	5
70	Thermodynamically Driven Formation of Intercalated Cu Carpets from Supported Cu Pyramids on MoS₂. Journal of Physical Chemistry Letters, 2022, 13, 6651-6656.	4.6	5
71	Adsorption and Diffusion of Gallium Adatoms on the Si(100)-2 Ã— 1 Reconstructed Surface: A Multiconfiguration Self-Consistent Field Study Utilizing Molecular Surface Clusters. Journal of Physical Chemistry C, 2011, 115, 23488-23500.	3.1	4
72	Analytic formulations for one-dimensional decay of rectangular homoepitaxial islands during coarsening on anisotropic fcc (110) surfaces. Physical Review B, 2013, 88, .	3.2	4

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73	Submonolayer Ag films on Fe(100): A first-principles analysis of energetics controlling adlayer thermodynamics and kinetics. Physical Review B, 2016, 93, .	3.2	4
74	Tailoring Kinetics on a Topological Insulator Surface by Defect-Induced Strain: Pb Mobility on Bi₂Te₃. Nano Letters, 2016, 16, 4454-4461.	9.1	4
75	Discontinuous Phase Transitions in Nonlocal Schloegl Models for Autocatalysis: Loss and Reemergence of a Nonequilibrium Gibbs Phase Rule. Physical Review Letters, 2018, 121, 120603.	7.8	4
76	Energy barriers for Pb adatom diffusion on stepped ultrathin Pb(111) quantum nanofilms: First-principles calculations. Physical Review B, 2019, 100, .	3.2	4
77	Surface structure of linear nanopores in amorphous silica: Comparison of properties for different pore generation algorithms. Journal of Chemical Physics, 2020, 153, 124708.	3.0	4
78	Tricriticality in generalized Schloegl models for autocatalysis: Lattice-gas realization with particle diffusion. Physica A: Statistical Mechanics and Its Applications, 2012, 391, 633-646.	2.6	3
79	Modeling of Diffusivity for 2D Vacancy Nanopits and Comparison with 2D Adatom Nanoislands on Metal(100) Surfaces Including Analysis for Ag(100). Journal of Physical Chemistry C, 2018, 122, 11334-11344.	3.1	3
80	Complex oscillatory decrease with size in diffusivity of {100}-epitaxially supported 3D fcc metal nanoclusters. Nanoscale, 2019, 11, 17506-17516.	5.6	3
81	Extended families of critical and stationary droplets for nonequilibrium phase transitions in spatially discrete bistable systems. Physical Review E, 2020, 101, 022803.	2.1	3
82	Enhanced Nanostructure Dynamics on Au(111) with Adsorbed Sulfur due to Auâ˜S Complex Formation. ChemPhysChem, 2021, 22, 349-358.	2.1	3
83	Molecular interactions in diffusion-controlled aldol condensation with mesoporous silica nanoparticles. Physical Chemistry Chemical Physics, 2022, 24, 10475-10487.	2.8	3
84	Catalytic conversion in nanoporous materials: Concentration oscillations and spatial correlations due to inhibited transport and intermolecular interactions. Journal of Chemical Physics, 2016, 145, 174705.	3.0	2
85	Catalytic conversion reactions in nanoporous systems with concentration-dependent selectivity: Statistical mechanical modeling. Physical Review E, 2016, 93, 052137.	2.1	2
86	Tracer counterpermeation analysis of diffusivity in finite-length nanopores with and without single-file dynamics. Physical Review E, 2017, 95, 012132.	2.1	2
87	Strainâ€Enhanced Metallic Intermixing in Shapeâ€Controlled Multilayered Coreâ€“Shell Nanostructures: Toward Shaped Intermetallics. Angewandte Chemie, 2020, 132, 10661-10667.	2.0	2
88	Shape Stability of Truncated Octahedral fcc Metal Nanocrystals. ACS Applied Materials & Interfaces, 2021, 13, 51954-51961.	8.0	2
89	Equilibrium shapes of facetted 3D metal nanoclusters intercalated near the surface of layered materials. Journal of Physics Condensed Matter, 2020, 32, 445001.	1.8	2
90	Boundary Conditions for Diffusion-Mediated Processes within Linear Nanopores: Exact Treatment of Coupling to an Equilibrated External Fluid. Journal of Physical Chemistry C, 2017, 121, 8873-8888.	3.1	1

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91	Generalized hydrodynamic analysis of transport through a finite open nanopore for two-component single-file systems. Physical Review E, 2020, 101, 062103.	2.1	1
92	Phase transitions in Schloegl's second model for autocatalysis on a Bethe lattice. Physical Review E, 2021, 104, 014135.	2.1	1
93	Sulfur-enhanced dynamics of coinage metal(111) surfaces: Step edges versus terraces as locations for metal-sulfur complex formation. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2022, 40, 023205.	2.1	1
94	Rotational and translational diffusion of liquid n-hexane: EFP-based molecular dynamics analysis. Journal of Chemical Physics, 2022, 156, 114503.	3.0	1
95	Atomistic and Coarse-Grained Modeling Strategies for Thin Film Nucleation and Growth on Quasicrystalline Surfaces. Materials Research Society Symposia Proceedings, 2013, 1517, 1.	0.1	0
96	Enhanced Nanostructure Dynamics on Au(111) with Adsorbed Sulfur due to Auâ^'S Complex Formation. ChemPhysChem, 2021, 22, 343-343.	2.1	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. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2022, 40, 031601.	2.1	0
99	Modeling of linear nanopores in a-SiO2 tuning pore surface structure. Microporous and Mesoporous Materials, 2022, , 112077.	4.4	0