Erik C. Neyts

List of Publications by Year
in descending order

182 papers	9,624 citations	53751 45 h-index	42364 92 g-index
187 all docs	187 docs citations	187 times ranked	8670 citing authors

#	Article	IF	Citations
1	Plasma-Catalytic Methanol Synthesis from CO₂ Hydrogenation over a Supported Cu Cluster Catalyst: Insights into the Reaction Mechanism. ACS Catalysis, 2022, 12, 1326-1337.	5.5	50
2	Indentation of graphene nano-bubbles. Nanoscale, 2022, , .	2.8	2
3	Foundations of plasma catalysis for environmental applications. Plasma Sources Science and Technology, 2022, 31, 053002.	1.3	28
4	Distribution Pattern of Metal Atoms in Bimetal-Doped Pyridinicâ€“N₄ Pores Determines Their Potential for Electrocatalytic N₂ Reduction. Journal of Physical Chemistry A, 2022, 126, 3080-3089.	1.1	0
5	Identification of a Robust and Durable FeN₄C_x Catalyst for ORR in PEM Fuel Cells and the Role of the Fifth Ligand. ACS Catalysis, 2022, 12, 7541-7549.	5.5	30
6	On the kinetics and equilibria of plasma-based dry reforming of methane. Chemical Engineering Journal, 2021, 405, 126630.	6.6	30
7	Entropic and enthalpic factors determining the thermodynamics and kinetics of carbon segregation from transition metal nanoparticles. Carbon, 2021, 171, 806-813.	5.4	5
8	Mechanisms of selective nanocarbon synthesis inside carbon nanotubes. Carbon, 2021, 171, 72-78.	5.4	3
9	Reactive plasma cleaning and restoration of transition metal dichalcogenide monolayers. Npj 2D Materials and Applications, 2021, 5, .	3.9	19
10	Effect of chemical modification on electronic transport properties of carbyne. Journal of Computational Electronics, 2021, 20, 848-854.	1.3	4
11	Contrasting H-Etching to OH-Etching in Plasma-Assisted Nucleation of Carbon Nanotubes. Journal of Physical Chemistry C, 2021, 125, 7849-7855.	1.5	1
12	Quantifying the impact of vibrational nonequilibrium in plasma catalysis: insights from a molecular dynamics model of dissociative chemisorption. Journal Physics D: Applied Physics, 2021, 54, 394004.	1.3	4
13	Linking Bi-Metal Distribution Patterns in Porous Carbon Nitride Fullerene to Its Catalytic Activity toward Gas Adsorption. Nanomaterials, 2021, 11, 1794.	1.9	6
14	DFT and Microkinetic Comparison of Ru-Doped Porphyrin-like Graphene and Nanotubes toward Catalytic Formic Acid Decomposition and Formation. Journal of Physical Chemistry C, 2021, 125, 18673-18683.	1.5	4
15	Breakdown of Universal Scaling for Nanometer-Sized Bubbles in Graphene. Nano Letters, 2021, 21, 8103-8110.	4.5	23
16	Plasma Catalysis for Ammonia Synthesis: A Microkinetic Modeling Study on the Contributions of Eleyâ€“Rideal Reactions. ACS Sustainable Chemistry and Engineering, 2021, 9, 13151-13163.	3.2	45
17	Enhanced piezoresponse and surface electric potential of hybrid biodegradable polyhydroxybutyrate scaffolds functionalized with reduced graphene oxide for tissue engineering. Nano Energy, 2021, 89, 106473.	8.2	28
18	Reaction mechanisms of C(3PJ) and C+(2PJ) with benzene in the interstellar medium from quantum mechanical molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 4205-4216.	1.3	2

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19	Plasma-Catalytic Ammonia Reforming of Methane over Cu-Based Catalysts for the Production of HCN and H₂ at Reduced Temperature. ACS Catalysis, 2021, 11, 1765-1773.	5.5	29
20	Ensemble-Based Molecular Simulation of Chemical Reactions under Vibrational Nonequilibrium. Journal of Physical Chemistry Letters, 2020, 11, 401-406.	2.1	7
21	Effect of van der Waals interactions on the adhesion strength at the interface of the hydroxyapatiteâ€“titanium biocomposite: a first-principles study. RSC Advances, 2020, 10, 37800-37805.	1.7	3
22	Ab initio calculations and a scratch test study of RF-magnetron sputter deposited hydroxyapatite and silicon-containing hydroxyapatite coatings. Surfaces and Interfaces, 2020, 21, 100727.	1.5	7
23	Free energy barriers from biased molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 114118.	1.2	24
24	Modeling the Physicochemical Properties of Natural Deep Eutectic Solvents. ChemSusChem, 2020, 13, 3789-3804.	3.6	84
25	Activation of CO₂ on Copper Surfaces: The Synergy between Electric Field, Surface Morphology, and Excess Electrons. Journal of Physical Chemistry C, 2020, 124, 6747-6755.	1.5	33
26	Predicted Influence of Plasma Activation on Nonoxidative Coupling of Methane on Transition Metal Catalysts. ACS Sustainable Chemistry and Engineering, 2020, 8, 6043-6054.	3.2	38
27	Direct oxidation of methane to methanol on Co embedded N-doped graphene: Comparing the role of N2O and O2 as oxidants. Applied Catalysis A: General, 2020, 602, 117716.	2.2	11
28	Accelerated molecular dynamics simulation of large systems with parallel collective variable-driven hyperdynamics. Computational Materials Science, 2020, 177, 109581.	1.4	13
29	Catalyzed growth of encapsulated carbyne. Carbon, 2019, 153, 1-5.	5.4	11
30	Direct methane conversion to methanol on M and MN4 embedded graphene (Mâ€¯=â€¯Ni and Si): A comparative DFT study. Applied Surface Science, 2019, 496, 143618.	3.1	35
31	Molecular evidence for feedstock-dependent nucleation mechanisms of CNTs. Nanoscale Horizons, 2019, 4, 674-682.	4.1	11
32	How process parameters and packing materials tune chemical equilibrium and kinetics in plasma-based CO2 conversion. Chemical Engineering Journal, 2019, 372, 1253-1264.	6.6	56
33	Special Issue on future directions in plasma nanoscience. Frontiers of Chemical Science and Engineering, 2019, 13, 199-200.	2.3	3
34	A route towards the fabrication of 2D heterostructures using atomic layer etching combined with selective conversion. 2D Materials, 2019, 6, 035030.	2.0	6
35	Molecular dynamics simulations of initial Pd and PdO nanocluster growth in a magnetron gas aggregation source. Frontiers of Chemical Science and Engineering, 2019, 13, 324-329.	2.3	10
36	Overcoming Old Scaling Relations and Establishing New Correlations in Catalytic Surface Chemistry: Combined Effect of Charging and Doping. Journal of Physical Chemistry C, 2019, 123, 6141-6147.	1.5	11

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37	CO₂ Activation on TiO₂-Supported Cu₅ and Ni₅ Nanoclusters: Effect of Plasma-Induced Surface Charging. Journal of Physical Chemistry C, 2019, 123, 6516-6525.	1.5	27
38	Effects of silicon doping on strengthening adhesion at the interface of the hydroxyapatiteâ€“titanium biocomposite: A first-principles study. Computational Materials Science, 2019, 159, 228-234.	1.4	14
39	Plasma Catalysis Modeling. Springer Series on Atomic, Optical, and Plasma Physics, 2019, , 69-114.	0.1	0
40	The role of healed N-vacancy defective BC2N sheet and nanotube by NO molecule in oxidation of NO and CO gas molecules. Surface Science, 2018, 672-673, 39-46.	0.8	5
41	High Coke Resistance of a TiO₂ Anatase (001) Catalyst Surface during Dry Reforming of Methane. Journal of Physical Chemistry C, 2018, 122, 9389-9396.	1.5	7
42	A comparative DFT study on CO oxidation reaction over Si-doped BC2N nanosheet and nanotube. Applied Surface Science, 2018, 439, 934-945.	3.1	24
43	Catalyst Preparation with Plasmas: How Does It Work?. ACS Catalysis, 2018, 8, 2093-2110.	5.5	323
44	Effect of plasma-induced surface charging on catalytic processes: application to CO₂activation. Plasma Sources Science and Technology, 2018, 27, 024001.	1.3	51
45	Enhancement of plasma generation in catalyst pores with different shapes. Plasma Sources Science and Technology, 2018, 27, 055008.	1.3	26
46	Modelling molecular adsorption on charged or polarized surfaces: a critical flaw in common approaches. Physical Chemistry Chemical Physics, 2018, 20, 8456-8459.	1.3	24
47	Plasma Technology: An Emerging Technology for Energy Storage. ACS Energy Letters, 2018, 3, 1013-1027.	8.8	363
48	The conversion mechanism of amorphous silicon to stoichiometric WS₂. Journal of Materials Chemistry C, 2018, 6, 4122-4130.	2.7	9
49	Atomistic simulations of plasma catalytic processes. Frontiers of Chemical Science and Engineering, 2018, 12, 145-154.	2.3	12
50	Mechanisms of elementary hydrogen ion-surface interactions during multilayer graphene etching at high surface temperature as a function of flux. Carbon, 2018, 137, 527-532.	5.4	10
51	Thermal recrystallization of short-range ordered WS2 films. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2018, 36, .	0.9	7
52	Understanding the Effect of Iodide Ions on the Morphology of Gold Nanorods. Particle and Particle Systems Characterization, 2018, 35, 1800051.	1.2	6
53	Two-dimensional WS₂nanoribbon deposition by conversion of pre-patterned amorphous silicon. Nanotechnology, 2017, 28, 04LT01.	1.3	18
54	Hampering Effect of Cholesterol on the Permeation of Reactive Oxygen Species through Phospholipids Bilayer: Possible Explanation for Plasma Cancer Selectivity. Scientific Reports, 2017, 7, 39526.	1.6	76

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55	DFT study of Ni-catalyzed plasma dry reforming of methane. Applied Catalysis B: Environmental, 2017, 205, 605-614.	10.8	57
56	Atomic scale behavior of oxygen-based radicals in water. Journal Physics D: Applied Physics, 2017, 50, 11LT01.	1.3	19
57	Synergistic effect of electric field and lipid oxidation on the permeability of cell membranes. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 839-847.	1.1	116
58	Mechanisms of Peptide Oxidation by Hydroxyl Radicals: Insight at the Molecular Scale. Journal of Physical Chemistry C, 2017, 121, 5787-5799.	1.5	18
59	Sulfur-alloyed Cr₂O₃: a new p-type transparent conducting oxide host. RSC Advances, 2017, 7, 4453-4459.	1.7	9
60	Toward the Understanding of Selective Si Nano-Oxidation by Atomic Scale Simulations. Accounts of Chemical Research, 2017, 50, 796-804.	7.6	16
61	Concurrent effects of wafer temperature and oxygen fraction on cryogenic silicon etching with SF₆/O₂ plasmas. Plasma Processes and Polymers, 2017, 14, 1700018.	1.6	9
62	Nanoscale mechanisms of CNT growth and etching in plasma environment. Journal Physics D: Applied Physics, 2017, 50, 184001.	1.3	14
63	Phosphatidylserine flipâ€flop induced by oxidation of the plasma membrane: a better insight by atomic scale modeling. Plasma Processes and Polymers, 2017, 14, 1700013.	1.6	18
64	Atomic-scale mechanisms of plasma-assisted elimination of nascent base-grown carbon nanotubes. Carbon, 2017, 118, 452-457.	5.4	5
65	Effect of electric fields on plasma catalytic hydrocarbon oxidation from atomistic simulations. Plasma Processes and Polymers, 2017, 14, 1600158.	1.6	7
66	How the alignment of adsorbed ortho H pairs determines the onset of selective carbon nanotube etching. Nanoscale, 2017, 9, 1653-1661.	2.8	9
67	Atomistic simulations of graphite etching at realistic time scales. Chemical Science, 2017, 8, 7160-7168.	3.7	6
68	The formation of Cr2O3 nanoclusters over graphene sheet and carbon nanotubes. Chemical Physics Letters, 2017, 687, 188-193.	1.2	5
69	Effect of head group and lipid tail oxidation in the cell membrane revealed through integrated simulations and experiments. Scientific Reports, 2017, 7, 5761.	1.6	88
70	A first principles study of p-type defects in LaCrO₃. Physical Chemistry Chemical Physics, 2017, 19, 22870-22876.	1.3	18
71	A DFT study of H-dissolution into the bulk of a crystalline Ni(111) surface: a chemical identifier for the reaction kinetics. Physical Chemistry Chemical Physics, 2017, 19, 19150-19158.	1.3	29
72	Stabilities of Bimetallic Nanoparticles for Chirality-Selective Carbon Nanotube Growth and the Effect of Carbon Interstitials. Journal of Physical Chemistry C, 2017, 121, 15430-15436.	1.5	3

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73	Density Functional Theory Study of Interface Interactions in Hydroxyapatite/Rutile Composites for Biomedical Applications. Journal of Physical Chemistry C, 2017, 121, 15687-15695.	1.5	16
74	Molecular Dynamics Simulations for Plasmaâ€Surface Interactions. Plasma Processes and Polymers, 2017, 14, 1600145.	1.6	53
75	Structural modification of P-glycoprotein induced by OH radicals: Insights from atomistic simulations. Scientific Reports, 2016, 6, 19466.	1.6	11
76	Elucidating the effects of gas flow rate on an SF6inductively coupled plasma and on the silicon etch rate, by a combined experimental and theoretical investigation. Journal Physics D: Applied Physics, 2016, 49, 385201.	1.3	1
77	How Oxygen Vacancies Activate CO₂ Dissociation on TiO₂ Anatase (001). Journal of Physical Chemistry C, 2016, 120, 21659-21669.	1.5	141
78	Plasmaâ€“liquid interactions: a review and roadmap. Plasma Sources Science and Technology, 2016, 25, 053002.	1.3	1,111
79	van der Waals density functionals applied to corundum-type sesquioxides: bulk properties and adsorption of CH₃ and C₆H₆ on (0001) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 23139-23146.	1.3	7
80	Direct observation of realistic-temperature fuel combustion mechanisms in atomistic simulations. Chemical Science, 2016, 7, 5280-5286.	3.7	56
81	Influence of the Material Dielectric Constant on Plasma Generation inside Catalyst Pores. Journal of Physical Chemistry C, 2016, 120, 25923-25934.	1.5	82
82	Multi-level molecular modelling for plasma medicine. Journal Physics D: Applied Physics, 2016, 49, 054002.	1.3	26
83	Can plasma be formed in catalyst pores? A modeling investigation. Applied Catalysis B: Environmental, 2016, 185, 56-67.	10.8	162
84	Selective Plasma Oxidation of Ultrasmall Si Nanowires. Journal of Physical Chemistry C, 2016, 120, 472-477.	1.5	4
85	Multilayer MoS₂ growth by metal and metal oxide sulfurization. Journal of Materials Chemistry C, 2016, 4, 1295-1304.	2.7	57
86	Size-dependent strain and surface energies of gold nanoclusters. Physical Chemistry Chemical Physics, 2016, 18, 792-800.	1.3	65
87	Plasma-Surface Interactions in Plasma Catalysis. Plasma Chemistry and Plasma Processing, 2016, 36, 185-212.	1.1	155
88	Effect of lipid peroxidation on membrane permeability of cancer and normal cells subjected to oxidative stress. Chemical Science, 2016, 7, 489-498.	3.7	307
89	A comparative study for the inactivation of multidrug resistance bacteria using dielectric barrier discharge and nano-second pulsed plasma. Scientific Reports, 2015, 5, 13849.	1.6	73
90	Atomic-scale insight into the interactions between hydroxyl radicals and DNA in solution using the ReaxFF reactive force field. New Journal of Physics, 2015, 17, 103005.	1.2	37

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91	Atomic scale simulation of carbon nanotube nucleation from hydrocarbon precursors. Nature Communications, 2015, 6, 10306.	5.8	61
92	The role of ions in plasma catalytic carbon nanotube growth: A review. Frontiers of Chemical Science and Engineering, 2015, 9, 154-162.	2.3	10
93	How do plasma-generated OH radicals react with biofilm components? Insights from atomic scale simulations. Biointerphases, 2015, 10, .	0.6	19
94	Molecular dynamics simulations of supported metal nanocatalyst formation by plasma sputtering. Catalysis Today, 2015, 256, 3-12.	2.2	30
95	Structural modification of the skin barrier by OH radicals: a reactive molecular dynamics study for plasma medicine. Journal Physics D: Applied Physics, 2015, 48, 155202.	1.3	30
96	Nanoscale thermodynamic aspects of plasma catalysis. Catalysis Today, 2015, 256, 23-28.	2.2	22
97	Thermal conductivity of titanium nitride/titanium aluminum nitride multilayer coatings deposited by lateral rotating cathode arc. Thin Solid Films, 2015, 578, 133-138.	0.8	72
98	Kinetics of Energy Selective Cs Encapsulation in Single-Walled Carbon Nanotubes for Damage-Free and Position-Selective Doping. Journal of Physical Chemistry C, 2015, 119, 11903-11908.	1.5	5
99	Adsorption of C and CH_x Radicals on Anatase (001) and the Influence of Oxygen Vacancies. Journal of Physical Chemistry C, 2015, 119, 4908-4921.	1.5	19
100	Integrated atomistic chemical imaging and reactive force field molecular dynamic simulations on silicon oxidation. Applied Physics Letters, 2015, 106, 011602.	1.5	21
101	Merging Metadynamics into Hyperdynamics: Accelerated Molecular Simulations Reaching Time Scales from Microseconds to Seconds. Journal of Chemical Theory and Computation, 2015, 11, 4545-4554.	2.3	86
102	Plasma Catalysis: Synergistic Effects at the Nanoscale. Chemical Reviews, 2015, 115, 13408-13446.	23.0	537
103	Inactivation of the Endotoxic Biomolecule Lipid A by Oxygen Plasma Species: A Reactive Molecular Dynamics Study. Plasma Processes and Polymers, 2015, 12, 162-171.	1.6	43
104	Efficient amorphous platinum catalyst cluster growth on porous carbon: A combined molecular dynamics and experimental study. Applied Catalysis B: Environmental, 2015, 162, 21-26.	10.8	24
105	Special issue on fundamentals of plasmaâ€“surface interactions. Journal Physics D: Applied Physics, 2014, 47, 220301.	1.3	4
106	On the time scale associated with Monte Carlo simulations. Journal of Chemical Physics, 2014, 141, 204104.	1.2	47
107	Fluorineâ€“Silicon Surface Reactions during Cryogenic and Near Room Temperature Etching. Journal of Physical Chemistry C, 2014, 118, 30315-30324.	1.5	26
108	Incorporation of Fluorescent Dyes in Atmospheric Pressure Plasma Coatings for In-Line Monitoring of Coating Homogeneity. Plasma Processes and Polymers, 2014, 11, 678-684.	1.6	4

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109	Combining molecular dynamics with Monte Carlo simulations: implementations and applications. Highlights in Theoretical Chemistry, 2014, , 277-288.	0.0	5
110	Interactions of plasma species on nickel catalysts: A reactive molecular dynamics study on the influence of temperature and surface structure. Applied Catalysis B: Environmental, 2014, 154-155, 1-8.	10.8	35
111	Reactive molecular dynamics simulations of oxygen species in a liquid water layer of interest for plasma medicine. Journal Physics D: Applied Physics, 2014, 47, 025205.	1.3	97
112	Understanding plasma catalysis through modelling and simulationâ€"a review. Journal Physics D: Applied Physics, 2014, 47, 224010.	1.3	241
113	Understanding polyethylene surface functionalization by an atmospheric He/O₂plasma through combined experiments and simulations. Journal Physics D: Applied Physics, 2014, 47, 224007.	1.3	29
114	Computer simulations of plasmaâ€"biomolecule and plasmaâ€"tissue interactions for a better insight in plasma medicine. Journal Physics D: Applied Physics, 2014, 47, 293001.	1.3	39
115	Thermodynamics at the nanoscale: phase diagrams of nickelâ€"carbon nanoclusters and equilibrium constants for phase transitions. Nanoscale, 2014, 6, 11981-11987.	2.8	29
116	Microscopic mechanisms of vertical graphene and carbon nanotube cap nucleation from hydrocarbon growth precursors. Nanoscale, 2014, 6, 9206-9214.	2.8	31
117	Ion irradiation for improved graphene network formation in carbon nanotube growth. Carbon, 2014, 77, 790-795.	5.4	9
118	Reactive Molecular Dynamics Simulations for a Better Insight in Plasma Medicine. Plasma Processes and Polymers, 2014, 11, 1156-1168.	1.6	48
119	Development of a ReaxFF reactive force field for intrinsic point defects in titanium dioxide. Computational Materials Science, 2014, 95, 579-591.	1.4	33
120	On the low-temperature growth mechanism of single walled carbon nanotubes in plasma enhanced chemical vapor deposition. Chemical Physics Letters, 2013, 590, 131-135.	1.2	18
121	Plasma enhanced growth of single walled carbon nanotubes at low temperature: A reactive molecular dynamics simulation. Carbon, 2013, 65, 269-276.	5.4	24
122	Interaction of O and OH radicals with a simple model system for lipids in the skin barrier: a reactive molecular dynamics investigation for plasma medicine. Journal Physics D: Applied Physics, 2013, 46, 395201.	1.3	69
123	Stability of Si epoxide defects in Si nanowires: a mixed reactive force field/DFT study. Physical Chemistry Chemical Physics, 2013, 15, 15091.	1.3	3
124	Reactive molecular dynamics simulations on SiO₂-coated ultra-small Si-nanowires. Nanoscale, 2013, 5, 719-725.	2.8	21
125	Temperature influence on the reactivity of plasma species on a nickel catalyst surface: An atomic scale study. Catalysis Today, 2013, 211, 131-136.	2.2	35
126	Combining molecular dynamics with Monte Carlo simulations: implementations and applications. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	51

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127	Plasma-Induced Destruction of Bacterial Cell Wall Components: A Reactive Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2013, 117, 5993-5998.	1.5	136
128	Atomistic modelling of CVD synthesis of carbon nanotubes and graphene. Nanoscale, 2013, 5, 6662.	2.8	88
129	New Mechanism for Oxidation of Native Silicon Oxide. Journal of Physical Chemistry C, 2013, 117, 9819-9825.	1.5	33
130	Formation of single layer graphene on nickel under far-from-equilibrium high flux conditions. Nanoscale, 2013, 5, 7250.	2.8	33
131	Plasma nanoscience: from nano-solids in plasmas to nano-plasmas in solids. Advances in Physics, 2013, 62, 113-224.	35.9	486
132	Defect Healing and Enhanced Nucleation of Carbon Nanotubes by Low-Energy Ion Bombardment. Physical Review Letters, 2013, 110, 065501.	2.9	65
133	Modeling the Growth of SWNTs and Graphene on the Atomic Scale. ECS Transactions, 2012, 45, 73-78.	0.3	2
134	On the c-Si|a-SiO₂ Interface in Hyperthermal Si Oxidation at Room Temperature. Journal of Physical Chemistry C, 2012, 116, 21856-21863.	1.5	35
135	Self-Limiting Oxidation in Small-Diameter Si Nanowires. Chemistry of Materials, 2012, 24, 2141-2147.	3.2	63
136	PECVD growth of carbon nanotubes: From experiment to simulation. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2012, 30, .	0.6	44
137	Plasma Species Interacting with Nickel Surfaces: Toward an Atomic Scale Understanding of Plasma-Catalysis. Journal of Physical Chemistry C, 2012, 116, 20958-20965.	1.5	52
138	Establishing Uniform Acceptance in Force Biased Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2012, 8, 1865-1869.	2.3	32
139	Modeling of plasma and plasma-surface interactions for medical, environmental and nano applications. Journal of Physics: Conference Series, 2012, 399, 012011.	0.3	8
140	Grain size tuning of nanocrystalline chemical vapor deposited diamond by continuous electrical bias growth: Experimental and theoretical study. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 1675-1682.	0.8	33
141	Atomic-scale simulations of reactive oxygen plasma species interacting with bacterial cell walls. New Journal of Physics, 2012, 14, 093043.	1.2	77
142	Insights in the Plasma-Assisted Growth of Carbon Nanotubes through Atomic Scale Simulations: Effect of Electric Field. Journal of the American Chemical Society, 2012, 134, 1256-1260.	6.6	88
143	Hyperthermal Oxidation of Si(100)2Ã—1 Surfaces: Effect of Growth Temperature. Journal of Physical Chemistry C, 2012, 116, 8649-8656.	1.5	35
144	Uniform-acceptance force-bias Monte Carlo method with time scale to study solid-state diffusion. Physical Review B, 2012, 85, .	1.1	62

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145	Theoretical Investigation of Grain Size Tuning during Prolonged Bias-Enhanced Nucleation. Chemistry of Materials, 2011, 23, 1414-1423.	3.2	11
146	Can We Control the Thickness of Ultrathin Silica Layers by Hyperthermal Silicon Oxidation at Room Temperature?. Journal of Physical Chemistry C, 2011, 115, 24839-24848.	1.5	50
147	Computer modelling of the plasma chemistry and plasma-based growth mechanisms for nanostructured materials. Journal Physics D: Applied Physics, 2011, 44, 174030.	1.3	34
148	Hyperthermal Oxygen Interacting with Silicon Surfaces: Adsorption, Implantation, and Damage Creation. Journal of Physical Chemistry C, 2011, 115, 4818-4823.	1.5	33
149	Changing Chirality during Single-Walled Carbon Nanotube Growth: A Reactive Molecular Dynamics/Monte Carlo Study. Journal of the American Chemical Society, 2011, 133, 17225-17231.	6.6	129
150	A density-functional theory simulation of the formation of Ni-doped fullerenes by ion implantation. Carbon, 2011, 49, 1013-1017.	5.4	20
151	Bond switching regimes in nickel and nickelâ€“carbon nanoclusters. Chemical Physics Letters, 2010, 488, 202-205.	1.2	22
152	Modeling of the plasma chemistry and plasmaâ€“surface interactions in reactive plasmas. Pure and Applied Chemistry, 2010, 82, 1283-1299.	0.9	22
153	Molecular dynamics simulations of Cl+ etching on a Si(100) surface. Journal of Applied Physics, 2010, 107, 113305.	1.1	25
154	Insights into the Growth of (Ultra)nanocrystalline Diamond by Combined Molecular Dynamics and Monte Carlo Simulations. Crystal Growth and Design, 2010, 10, 3005-3021.	1.4	17
155	Differences between Ultrananocrystalline and Nanocrystalline Diamond Growth: Theoretical Investigation of C_xH_y Species at Diamond Step Edges. Crystal Growth and Design, 2010, 10, 4123-4134.	1.4	17
156	Catalyzed Growth of Carbon Nanotube with Definable Chirality by Hybrid Molecular Dynamicsâ˜Force Biased Monte Carlo Simulations. ACS Nano, 2010, 4, 6665-6672.	7.3	162
157	Computer Modeling of Plasmas and Plasmaâ€Surface Interactions. Plasma Processes and Polymers, 2009, 6, 295-307.	1.6	32
158	Formation of endohedral Ni@C60 and exohedral Niâ€“C60 metallofullerene complexes by simulated ion implantation. Carbon, 2009, 47, 1028-1033.	5.4	22
159	Numerical Study of the Size-Dependent Melting Mechanisms of Nickel Nanoclusters. Journal of Physical Chemistry C, 2009, 113, 2771-2776.	1.5	80
160	Numerical simulation of hydrocarbon plasmas for nanoparticle formation and the growth of nanostructured thin films. Plasma Physics and Controlled Fusion, 2009, 51, 124034.	0.9	2
161	Modeling adatom surface processes during crystal growth: A new implementation of the Metropolis Monte Carlo algorithm. CrystEngComm, 2009, 11, 1597.	1.3	19
162	MODELING PECVD GROWTH OF NANOSTRUCTURED CARBON MATERIALS. High Temperature Material Processes, 2009, 13, 399-412.	0.2	1

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163	Molecular Dynamics Simulations of the Sticking and Etch Behavior of Various Growth Species of (Ultra)Nanocrystalline Diamond Films. Chemical Vapor Deposition, 2008, 14, 213-223.	1.4	35
164	Study of Atmospheric MOCVD of TiO₂ Thin Films by Means of Computational Fluid Dynamics Simulations. Chemical Vapor Deposition, 2008, 14, 339-346.	1.4	15
165	On the reaction behaviour of hydrocarbon species at diamond (1â€‰0â€‰0) and (1â€‰1â€‰1) surfaces: a molecular dynamics investigation. Journal Physics D: Applied Physics, 2008, 41, 032006.	1.3	22
166	Reaction mechanisms and thin a-C:H film growth from low energy hydrocarbon radicals. Journal of Physics: Conference Series, 2007, 86, 012020.	0.3	19
167	Molecular Dynamics Simulations of the Growth of Thin Aâ€C:H Films Under Additional Ion Bombardment: Influence of the Growth Species and the Ar⁺ Ion Kinetic Energy. Chemical Vapor Deposition, 2007, 13, 312-318.	1.4	19
168	Macroscale computer simulations to investigate the chemical vapor deposition of thin metal-oxide films. Surface and Coatings Technology, 2007, 201, 8838-8841.	2.2	5
169	Reaction mechanisms of low-kinetic energy hydrocarbon radicals on typical hydrogenated amorphous carbon (a-C:H) sites: A molecular dynamics study. Diamond and Related Materials, 2006, 15, 1663-1676.	1.8	18
170	Effect of hydrogen on the growth of thin hydrogenated amorphous carbon films from thermal energy radicals. Applied Physics Letters, 2006, 88, 141922.	1.5	34
171	Influence of internal energy and impact angle on the sticking behaviour of reactive radicals in thin a-C:H film growth: a molecular dynamics study. Physical Chemistry Chemical Physics, 2006, 8, 2066.	1.3	9
172	Monte Carlo method for simulations of adsorbed atom diffusion on a surface. Diamond and Related Materials, 2006, 15, 1629-1635.	1.8	7
173	Computer Simulations for Processing Plasmas. Plasma Processes and Polymers, 2006, 3, 110-119.	1.6	13
174	The effect of hydrogen on the electronic and bonding properties of amorphous carbon. Journal of Physics Condensed Matter, 2006, 18, 10803-10815.	0.7	16
175	Unraveling the deposition mechanism in a-C:H thin-film growth: A molecular-dynamics study for the reaction behavior of C3 and C3H radicals with a-C:H surfaces. Journal of Applied Physics, 2006, 99, 014902.	1.1	24
176	Densification of thin a-Câ€‰:â€‰H films grown from low-kinetic energy hydrocarbon radicals under the influence of H and C particle fluxes: a molecular dynamics study. Journal Physics D: Applied Physics, 2006, 39, 1948-1953.	1.3	3
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178	Numerical modeling for a better understanding of gas discharge plasmas. High Temperature Material Processes, 2005, 9, 321-344.	0.2	1
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