Yong-Hyun Kim

List of Publications by Year
in descending order

128 papers	9,036 citations	41323 49 h-index	40954 93 g-index
130 all docs	130 docs citations	130 times ranked	13345 citing authors

#	Article	IF	Citations
1	Hydrogen Storage in Novel Organometallic Buckyballs. Physical Review Letters, 2005, 94, 155504.	2.9	629
2	Suppression of Hydrogen Evolution Reaction in Electrochemical N₂ Reduction Using Single-Atom Catalysts: A Computational Guideline. ACS Catalysis, 2018, 8, 7517-7525.	5.5	545
3	Single-atom catalysts for CO₂ electroreduction with significant activity and selectivity improvements. Chemical Science, 2017, 8, 1090-1096.	3.7	430
4	Chemical structures of hydrazine-treated graphene oxide and generation of aromatic nitrogen doping. Nature Communications, 2012, 3, 638.	5.8	354
5	Reversible Lithiumâ€Ion Insertion in Molybdenum Oxide Nanoparticles. Advanced Materials, 2008, 20, 3627-3632.	11.1	330
6	Theory, Synthesis, and Oxygen Reduction Catalysis of Fe-Porphyrin-Like Carbon Nanotube. Physical Review Letters, 2011, 106, 175502.	2.9	317
7	Nondissociative Adsorption ofH2Molecules in Light-Element-Doped Fullerenes. Physical Review Letters, 2006, 96, 016102.	2.9	305
8	Steric-Hindrance-Driven Shape Transition in PbS Quantum Dots: Understanding Size-Dependent Stability. Journal of the American Chemical Society, 2013, 135, 5278-5281.	6.6	301
9	Transparent Conductive Single-Walled Carbon Nanotube Networks with Precisely Tunable Ratios of Semiconducting and Metallic Nanotubes. ACS Nano, 2008, 2, 1266-1274.	7.3	297
10	Workfunction-Tunable, N-Doped Reduced Graphene Transparent Electrodes for High-Performance Polymer Light-Emitting Diodes. ACS Nano, 2012, 6, 159-167.	7.3	297
11	Tailored semiconducting carbon nanotube networks with enhanced thermoelectric properties. Nature Energy, 2016, 1, .	19.8	270
12	Enhanced Nanoscale Friction on Fluorinated Graphene. Nano Letters, 2012, 12, 6043-6048.	4.5	262
13	Effects of sulfur doping on graphene-based nanosheets for use as anode materials in lithium-ion batteries. Journal of Power Sources, 2014, 262, 79-85.	4.0	203
14	Ultrastable PbSe Nanocrystal Quantum Dots via in Situ Formation of Atomically Thin Halide Adlayers on PbSe(100). Journal of the American Chemical Society, 2014, 136, 8883-8886.	6.6	172
15	Solid State Enabled Reversible Four Electron Storage. Advanced Energy Materials, 2013, 3, 120-127.	10.2	155
16	Electronic structure of radially deformed BN andBC3nanotubes. Physical Review B, 2001, 63, .	1.1	149
17	Ambient Carbon Dioxide Capture by Boron-Rich Boron Nitride Nanotube. Journal of the American Chemical Society, 2011, 133, 2084-2087.	6.6	146
18	Enhancement of the anisotropic photocurrent in ferroelectric oxides by strain gradients. Nature Nanotechnology, 2015, 10, 972-979.	15.6	134

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19	Intrinsic Photoluminescence Emission from Subdomained Graphene Quantum Dots. Advanced Materials, 2016, 28, 5255-5261.	11.1	124
20	Nanotribological Properties of Fluorinated, Hydrogenated, and Oxidized Graphenes. Tribology Letters, 2013, 50, 137-144.	1.2	123
21	Band-gap modification by radial deformation in carbon nanotubes. Physical Review B, 1999, 60, 10656-10659.	1.1	116
22	Defective fullerenes and nanotubes as molecular magnets:â€‚Anab initiostudy. Physical Review B, 2003, 68, .	1.1	114
23	Dopant-specific unzipping of carbon nanotubes for intact crystalline graphene nanostructures. Nature Communications, 2016, 7, 10364.	5.8	109
24	Wiring-Up Hydrogenase with Single-Walled Carbon Nanotubes. Nano Letters, 2007, 7, 3528-3534.	4.5	106
25	Halideâ€“Amine Coâ€Passivated Indium Phosphide Colloidal Quantum Dots in Tetrahedral Shape. Angewandte Chemie - International Edition, 2016, 55, 3714-3718.	7.2	102
26	Divacancy-nitrogen-assisted transition metal dispersion and hydrogen adsorption in defective graphene: A first-principles study. Physical Review B, 2010, 81, .	1.1	90
27	Selective and Regenerative Carbon Dioxide Capture by Highly Polarizing Porous Carbon Nitride. ACS Nano, 2015, 9, 9148-9157.	7.3	88
28	Effect of Spin State on the Dihydrogen Binding Strength to Transition Metal Centers in Metal-Organic Frameworks. Journal of the American Chemical Society, 2007, 129, 12606-12607.	6.6	82
29	Halideâ€“Amine Coâ€Passivated Indium Phosphide Colloidal Quantum Dots in Tetrahedral Shape. Angewandte Chemie, 2016, 128, 3778-3782.	1.6	82
30	N2-dopant of graphene with electrochemically switchable bifunctional ORR/OER catalysis for Zn-air battery. Energy Storage Materials, 2020, 32, 517-524.	9.5	80
31	IIIâ€“V colloidal nanocrystals: control of covalent surfaces. Chemical Science, 2020, 11, 913-922.	3.7	77
32	Itinerant ferromagnetism in heterostructured C/BN nanotubes. Physical Review B, 2003, 67, .	1.1	75
33	Accurate and efficient calculation of van der Waals interactions within density functional theory by local atomic potential approach. Journal of Chemical Physics, 2008, 129, 154102.	1.2	73
34	Divalent Fe Atom Coordination in Two-Dimensional Microporous Graphitic Carbon Nitride. ACS Applied Materials & Interfaces, 2016, 8, 25438-25443.	4.0	70
35	Switching and Sensing Spin States of Coâ€“Porphyrin in Bimolecular Reactions on Au(111) Using Scanning Tunneling Microscopy. ACS Nano, 2013, 7, 9312-9317.	7.3	61
36	Spectral Correlation in Incommensurate Multiwalled Carbon Nanotubes. Physical Review Letters, 2003, 90, 026601.	2.9	60

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37	Self-catalyzed hydrogenation and dihydrogen adsorption on titanium carbide nanoparticles. Chemical Physics Letters, 2006, 425, 273-277.	1.2	60
38	Dynamics of Fullerene Coalescence. Physical Review Letters, 2003, 90, 065501.	2.9	59
39	Subband mixing rules in circumferentially perturbed carbon nanotubes: Effects of transverse electric fields. Physical Review B, 2001, 64, .	1.1	58
40	Monodisperse Pattern Nanoalloying for Synergistic Intermetallic Catalysis. Nano Letters, 2013, 13, 5720-5726.	4.5	58
41	Enhancement of Friction by Water Intercalated between Graphene and Mica. Journal of Physical Chemistry Letters, 2017, 8, 3482-3487.	2.1	57
42	First-Principles Theory of Electrochemical Capacitance of Nanostructured Materials: Dipole-Assisted Subsurface Intercalation of Lithium in Pseudocapacitive TiO₂ Anatase Nanosheets. Journal of Physical Chemistry C, 2011, 115, 4909-4915.	1.5	56
43	First-Principles Prediction of Icosahedral Quantum Dots for Tetravalent Semiconductors. Physical Review Letters, 2004, 93, .	2.9	55
44	Thermoelectric imaging of structural disorder in epitaxial graphene. Nature Materials, 2013, 12, 913-918.	13.3	55
45	Borane-modified graphene-based materials as CO2 adsorbents. Carbon, 2014, 79, 450-456.	5.4	53
46	Extremely Stable Luminescent Crosslinked Perovskite Nanoparticles under Harsh Environments over 1.5 Years. Advanced Materials, 2021, 33, e2005255.	11.1	53
47	High Performance Colloidal Quantum Dot Photovoltaics by Controlling Protic Solvents in Ligand Exchange. Advanced Energy Materials, 2017, 7, 1700301.	10.2	51
48	Carrier-mediated long-range ferromagnetism in electron-doped Fe-C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and Fe-N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>incorporated graphene. Physical Review B, 2012, 86, .	1.1	50
49	Ab initio design of Ca-decorated organic frameworks for high capacity molecular hydrogen storage with enhanced binding. Applied Physics Letters, 2009, 95, 033109.	1.5	49
50	Is the Chain of Oxidation and Reduction Process Reversible in Luminescent Graphene Quantum Dots?. Small, 2015, 11, 3773-3781.	5.2	49
51	Progress in Computational and Machineâ€Learning Methods for Heterogeneous Smallâ€Molecule Activation. Advanced Materials, 2020, 32, e1907865.	11.1	46
52	Complementary p- and n-Type Polymer Doping for Ambient Stable Graphene Inverter. ACS Nano, 2014, 8, 650-656.	7.3	42
53	Generation of Ultraâ€Highâ€Molecularâ€Weight Polyethylene from Metallocenes Immobilized onto Nâ€Doped Graphene Nanoplatelets. Macromolecular Rapid Communications, 2013, 34, 533-538.	2.0	40
54	Nanotube Wires on Commensurate InAs Surfaces: Binding Energies, Band Alignments, and Bipolar Doping by the Surfaces. Physical Review Letters, 2004, 92, 176102.	2.9	38

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55	Accuracy of density functional theory methods for weakly bonded systems: The case of dihydrogen binding on metal centers. Physical Review B, 2010, 82, .	1.1	38
56	Nanoscale Friction on Confined Water Layers Intercalated between MoS₂ Flakes and Silica. Journal of Physical Chemistry C, 2019, 123, 8827-8835.	1.5	36
57	Hole-Mediated Hydrogen Spillover Mechanism in Metal-Organic Frameworks. Physical Review Letters, 2010, 104, 236101.	2.9	34
58	Origin of the Stability and Transition from Anionic to Cationic Surface Ligand Passivation of All-Inorganic Cesium Lead Halide Perovskite Nanocrystals. Journal of Physical Chemistry Letters, 2020, 11, 652-658.	2.1	33
59	Seebeck Effect at the Atomic Scale. Physical Review Letters, 2014, 112, 136601.	2.9	32
60	Effect of chemical bonding on the magnetic stability and magnetic moment in Mn-based binary compounds. Physical Review B, 2005, 72, .	1.1	30
61	Ab initiocalculations predicting the existence of an oxidized calcium dihydrogen complex to store molecular hydrogen in densities up to 100 g/L. Physical Review B, 2009, 79, .	1.1	29
62	Persistent Medium-Range Order and Anomalous Liquid Properties ofAl1âˆ’xCuxAlloys. Physical Review Letters, 2012, 108, 115901.	2.9	29
63	The Effect of Thickness and Chemical Reduction of Graphene Oxide on Nanoscale Friction. Journal of Physical Chemistry B, 2018, 122, 543-547.	1.2	27
64	Self-Assembly of Linear Arrays of Semiconductor Nanoparticles on Carbon Single-Walled Nanotubesâ€. Journal of Physical Chemistry B, 2006, 110, 25153-25157.	1.2	26
65	Gold nanoparticle-doped graphene nanosheets: sub-nanosized gold clusters nucleate and grow at the nitrogen-induced defects on graphene surfaces. Journal of Materials Chemistry, 2012, 22, 7130.	6.7	26
66	Cyclodextrin driven hydrophobicâˆ•hydrophilic transformation of semiconductor nanoparticles. Applied Physics Letters, 2005, 86, 033108.	1.5	25
67	Atomically Abrupt Liquid-Oxide Interface Stabilized by Self-Regulated Interfacial Defects: The Case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Al</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mi>Al</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Interfaces. Physical Review Letters, 2012, 108, 226105.	2.9	25
68	Growth Mechanism of Catalyst-Free and Mask-Free Heteroepitaxial GaN Submicrometer- and Micrometer-Sized Rods under Biaxial Strain: Variation of Surface Energy and Adatom Kinetics. Crystal Growth and Design, 2012, 12, 3838-3844.	1.4	25
69	Finite-Temperature Hydrogen Adsorption and Desorption Thermodynamics Driven by Soft Vibration Modes. Physical Review Letters, 2013, 111, 066102.	2.9	25
70	Atomic models for anionic ligand passivation of cation-rich surfaces of IVâ€“VI, IIâ€“VI, and IIIâ€“V colloidal quantum dots. Chemical Communications, 2017, 53, 388-391.	2.2	25
71	Dielectric-screening properties and Coulomb pseudopotentialÎ¼*forMgB2. Physical Review B, 2004, 70, .	1.1	24
72	Opening space for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>Cointercalation of graphite with lithium and small organic molecules. Physical Review B, 2008, 78, .	1.1	24

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73	Origin of the Diverse Melting Behaviors of Intermediate-Size Nanoclusters: Theoretical Study of AlN(N= 51â^'58, 64). Journal of the American Chemical Society, 2010, 132, 18287-18291.	6.6	24
74	Isotope- and Thickness-Dependent Friction of Water Layers Intercalated Between Graphene and Mica. Tribology Letters, 2018, 66, 1.	1.2	24
75	>1000-Fold Lifetime Extension of a Nickel Electromechanical Contact Device via Graphene. ACS Applied Materials & Interfaces, 2018, 10, 9085-9093.	4.0	23
76	Anomalous Defect Dependence of Thermal Conductivity in Epitaxial WO₃ Thin Films. Advanced Materials, 2019, 31, e1903738.	11.1	23
77	Electronic structure of collapsed C, BN, and BC3 nanotubes. Current Applied Physics, 2001, 1, 39-44.	1.1	22
78	Slow colloidal growth of PbSe nanocrystals for facile morphology and size control. RSC Advances, 2014, 4, 9842.	1.7	22
79	Shape Control of Al Nanoclusters by Ligand Size. Journal of the American Chemical Society, 2009, 131, 8522-8526.	6.6	21
80	Enhanced dihydrogen adsorption in symmetry-lowered metalâ€"porphyrin-containing frameworks. Physical Chemistry Chemical Physics, 2009, 11, 11400.	1.3	21
81	Ni Nanoparticles on Ni Core/N-Doped Carbon Shell Heterostructures for Electrocatalytic Oxygen Evolution. ACS Applied Nano Materials, 2021, 4, 9418-9429.	2.4	21
82	Microscopic Theory of Hysteretic Hydrogen Adsorption in Nanoporous Materials. Journal of the American Chemical Society, 2010, 132, 1510-1511.	6.6	19
83	Selective engineering of oxygen-containing functional groups using the alkyl ligand oleylamine for revealing the luminescence mechanism of graphene oxide quantum dots. Nanoscale, 2017, 9, 18635-18643.	2.8	19
84	Derivation of a governing rule in triboelectric charging and series from thermoelectricity. Physical Review Research, 2022, 4, .	1.3	19
85	Comment on â€œInaccuracy of Density Functional Theory Calculations for Dihydrogen Binding Energetics onto Ca Cation Centersâ€• Physical Review Letters, 2010, 104, 179601; author reply 179602.	2.9	18
86	Harnessing the topotactic transition in oxide heterostructures for fast and high-efficiency electrochromic applications. Science Advances, 2020, 6, .	4.7	17
87	Tailored growth of single-crystalline InP tetrapods. Nature Communications, 2021, 12, 4454.	5.8	17
88	Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. Physical Review B, 2012, 85, .	1.1	16
89	O₂, NO₂ and NH₃ coordination to Co-porphyrin studied with scanning tunneling microscopy on Au(111). Nanoscale, 2019, 11, 8510-8517.	2.8	16
90	Tuning and sensing spin interactions in Co-porphyrin/Au with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2	1.1	15

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91	Amorphous Mixture of Two Indium-Free BaSnO₃ and ZnSnO₃ for Thin-Film Transistors with Balanced Performance and Stability. ACS Applied Materials & Interfaces, 2020, 12, 3719-3726.	4.0	15
92	Origin of Enhanced Dihydrogen-Metal Interaction in Carboxylate Bridged<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>â€“Paddle-Wheel Frameworks. Physical Review Letters, 2010, 105, 236105.	2.9	14
93	Half-Solidity of Tetrahedral-like Al₅₅ Clusters. ACS Nano, 2010, 4, 1092-1098.	7.3	14
94	First-Principles Study of Electronic Structure and Hydrogen Adsorption of 3d Transition Metal Exposed Paddle Wheel Frameworks. Journal of Physical Chemistry C, 2012, 116, 7386-7392.	1.5	14
95	Interfacial Thermal Conductance Observed to be Higher in Semiconducting than Metallic Carbon Nanotubes. ACS Nano, 2012, 6, 3853-3860.	7.3	14
96	Hysteresis and Photoinstability Caused by Mobile Ions in Colloidal Quantum Dot Photovoltaics. Journal of Physical Chemistry Letters, 2017, 8, 5259-5263.	2.1	14
97	Raman spectroscopy of charge transfer interactions between single wall carbon nanotubes and [FeFe] hydrogenase. Dalton Transactions, 2008, , 5454.	1.6	13
98	Visualizing tilted binding and precession of diatomic NO adsorbed to Co-porphyrin on Au(111) using scanning tunneling microscopy. Chemical Science, 2014, 5, 2224-2229.	3.7	13
99	Axial coordination and electronic structure of diatomic NO, CO, and O₂ molecules adsorbed onto Co-tetraphenylporphyrin on Au(111), Ag(111), and Cu(111): a density-functional theory study. Dalton Transactions, 2016, 45, 16673-16681.	1.6	13
100	Thickness-dependent photocatalytic performance of graphite oxide for degrading organic pollutants under visible light. Physical Chemistry Chemical Physics, 2016, 18, 10882-10886.	1.3	13
101	Coordination structure of Jacobsen catalyst with N-modified graphene and their electrocatalytic properties for reducing oxygen molecules. Applied Catalysis B: Environmental, 2020, 263, 118337.	10.8	13
102	Tip-Induced Strain Engineering of a Single Metal Halide Perovskite Quantum Dot. ACS Nano, 2021, 15, 9057-9064.	7.3	13
103	Probing Single-Molecule Dissociations from a Bimolecular Complex NOâ€“Co-Porphyrin. ACS Nano, 2015, 9, 7722-7728.	7.3	12
104	Hidden breathing kagome topology in hexagonal transition metal dichalcogenides. Physical Review B, 2022, 105, .	1.1	12
105	Dihydrogen bonding,p-type conductivity, and origin of change in work function of hydrogenated diamond (001) surfaces. Physical Review B, 2006, 74, .	1.1	10
106	Altering the spin state of transition metal centers in metalâ€“organic frameworks by molecular hydrogen adsorption: a first-principles study. Physical Chemistry Chemical Physics, 2011, 13, 5042.	1.3	10
107	Origin of High- T_C Ferromagnetism in Isovalent-Doped III-V Semiconductors. Physical Review Applied, 2019, 11, .	1.5	10
108	Tailoring graphene magnetism by zigzag triangular holes: A first-principles thermodynamics study. AIP Advances, 2016, 6, 035023.	0.6	9

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109	Shape-controlled syntheses of metal oxide nanoparticles by the introduction of rare-earth metals. Nanoscale, 2017, 9, 2732-2738.	2.8	9
110	First-principles calculation of thermodynamic stability of acids and bases under pH environment: A microscopic pH theory. Journal of Chemical Physics, 2012, 136, 134112.	1.2	8
111	Reversible oxidation states of single layer graphene tuned by electrostatic potential. Surface Science, 2013, 612, 37-41.	0.8	8
112	Bimodal Control of Heat Transport at Grapheneâ€“Metal Interfaces Using Disorder in Graphene. Scientific Reports, 2016, 6, 34428.	1.6	7
113	Microscopic States and the Verwey Transition of Magnetite Nanocrystals Investigated by Nuclear Magnetic Resonance. Nano Letters, 2018, 18, 1745-1750.	4.5	7
114	Growing extremely thin bulklike metal film on a semiconductor surface: Monolayer Al(111) on Si(111). Applied Physics Letters, 2007, 91, .	1.5	6
115	Origin of anomalous strain effects on the molecular adsorption on boron-doped graphene. Journal of Chemical Physics, 2013, 139, 044709.	1.2	6
116	Metal-induced n+/n homojunction for ultrahigh electron mobility transistors. NPG Asia Materials, 2020, 12, .	3.8	6
117	Influence of the metal phthalocyanine molecular orientation on charge separation at the organic donor/acceptor interface. Journal of Materials Chemistry C, 2021, 9, 2156-2164.	2.7	6
118	Assessing the Predictive Power of Density Functional Theory in Finite-Temperature Hydrogen Adsorption/Desorption Thermodynamics. Journal of Physical Chemistry C, 2018, 122, 26189-26195.	1.5	5
119	Quantitative Analysis of Calcium Phosphate Nanocluster Growth Using Time-of-Flight Medium-Energy-Ion-Scattering Spectroscopy. ACS Central Science, 2018, 4, 1253-1260.	5.3	5
120	Electron transport through quantum-dot states of n-type carbon nanotubes. Applied Physics Letters, 2002, 81, 2264-2266.	1.5	4
121	Spectral properties of incommensurate double-walled carbon nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2004, 22, 666-669.	1.3	2
122	Importance of Turning to Renewable Energy Resources with Hydrogen as a Promising Candidate and on-board Storage a Critical Barrier. Materials Research Society Symposia Proceedings, 2005, 895, 1.	0.1	2
123	Diversity of hole-trap centers due to small polarons and bipolarons in Ca-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>BiFe</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> : Origin of electrochromism. Physical Review B, 2020, 101, .	1.1	2
124	Cyclodextrins Stabilize TOPO-(CdSe)ZnS Quantum Dots In Water. Materials Research Society Symposia Proceedings, 2004, 823, W4.5.1.	0.1	0
125	Generalized Kubas Complexes as a Novel Means for Room Temperature Molecular Hydrogen Storage. Materials Research Society Symposia Proceedings, 2004, 837, 63.	0.1	0
126	Hydrogen Storage in Novel Carbon-Based Nanostructured Materials. Materials Research Society Symposia Proceedings, 2006, 927, 1.	0.1	0

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127	Novel Organometallic Fullerene Complexes for Vehicular Hydrogen Storage. Materials Research Society Symposia Proceedings, 2007, 1041, 1.	0.1	0
128	Perovskite Nanoparticles: Extremely Stable Luminescent Crosslinked Perovskite Nanoparticles under Harsh Environments over 1.5 Years (Adv. Mater. 3/2021). Advanced Materials, 2021, 33, 2170017.	11.1	0