List of Publications by Year in descending order

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WELCHEN

#	Article	IF	CITATIONS
1	A new MoCN monolayer containing stable cyano structural units as a high-efficiency catalyst for the hydrogen evolution reaction. Nanoscale, 2022, , .	2.8	1
2	Efficient, biosafe and tissue adhesive hemostatic cotton gauze with controlled balance of hydrophilicity and hydrophobicity. Nature Communications, 2022, 13, 552.	5.8	55
3	Realizing Efficient Catalytic Performance and High Selectivity for Oxygen Reduction Reaction on a 2D Ni ₂ SbTe ₂ Monolayer. Inorganic Chemistry, 2022, 61, 2284-2291.	1.9	7
4	Janus MoPC Monolayer with Superior Electrocatalytic Performance for the Hydrogen Evolution Reaction. ACS Applied Materials & amp; Interfaces, 2022, 14, 7836-7844.	4.0	13
5	High HER Catalytic Activity of Bulk GeP3 System and Its further Improvement by Introducing Monovacancy: A First-Principles Investigation. Journal of the Electrochemical Society, 2021, 168, 056508.	1.3	1
6	Probing the effect of carbon doping on structures, properties, and stability of magnesium clusters. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	3
7	Interface Engineering of Heterogeneous CeO ₂ –CoO Nanofibers with Rich Oxygen Vacancies for Enhanced Electrocatalytic Oxygen Evolution Performance. ACS Applied Materials & Interfaces, 2021, 13, 46998-47009.	4.0	40
8	Constructing a simple Cone–Chain motif to significantly enhance the first hyperpolarizability of horn-shaped carbon nanocones. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 136, 115021.	1.3	0
9	Increasing Silicon Concentration and Doping Heteroatom to Successfully Realize High HER Catalytic Activity in 2D Metal-Free BSi _n (n = 1–4) Structures: A First-Principles Study. Journal of the Electrochemical Society, 2021, 168, 126527.	1.3	3
10	The crucial role of strained ring in enhancing the hydrogen evolution catalytic activity for the 2D carbon allotropes: a high-throughput first-principles investigation. 2D Materials, 2020, 7, 015015.	2.0	22
11	Applying surface strain and coupling with pure or N/B-doped graphene to successfully achieve high HER catalytic activity in 2D layered SnP ₃ -based nanomaterials: a first-principles investigation. Inorganic Chemistry Frontiers, 2020, 7, 647-658.	3.0	22
12	Embedding tetrahedral 3d transition metal TM ₄ clusters into the cavity of two-dimensional graphdiyne to construct highly efficient and nonprecious electrocatalysts for hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2020, 22, 3254-3263.	1.3	20
13	Facile Strategy to Extend Stability of Simple Component-Alumina-Supported Palladium Catalysts for Efficient Methane Combustion. ACS Applied Materials & Interfaces, 2020, 12, 56095-56107.	4.0	36
14	Theoretical design of a series of 2D TM–C ₃ N ₄ and TM–C ₃ N ₄ @graphene (TM = V, Nb and Ta) nanostructures with highly efficient catalytic activity for the hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2019, 21, 1773-1783	1.3	27
15	Theoretical investigation on the structures, electronic and magnetic properties of new 2D/1D composite nanosystems by adsorbing superhalogen MnCl3 on the BN monolayer/nanoribbons. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	3
16	Theoretical investigation on the high HER catalytic activity of 2D layered GeP3 nanomaterials and its further enhancement by applying the surface strain or coupling with graphene. Applied Surface Science, 2019, 481, 272-280.	3.1	22
17	Theoretical predication of the high hydrogen evolution catalytic activity for the cubic and tetragonal SnP systems. Physical Chemistry Chemical Physics, 2019, 21, 5521-5530.	1.3	12
18	Adsorbing the magnetic superhalogen MnCl ₃ to realize intriguing half-metallic and spin-gapless-semiconducting behavior in zigzag or armchair SiC nanoribbon. RSC Advances, 2018, 8, 13167-13177.	1.7	6

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19	Highly efficient catalytic activity for the hydrogen evolution reaction on pristine and monovacancy defected WP systems: a first-principles investigation. Physical Chemistry Chemical Physics, 2018, 20, 13757-13764.	1.3	25
20	Theoretical insights into the effective hydrogen evolution on Cu3P and its evident improvement by surface-doped Ni atoms. Physical Chemistry Chemical Physics, 2018, 20, 10407-10417.	1.3	29
21	Host–Guest Interaction Creates Hydrogen-Evolution Electrocatalytic Active Sites in 3d Transition Metal-Intercalated Titanates. ACS Applied Materials & Interfaces, 2018, 10, 696-703.	4.0	17
22	Carbonâ€Encapsulated WO <i>_x</i> Hybrids as Efficient Catalysts for Hydrogen Evolution. Advanced Materials, 2018, 30, e1705979.	11.1	140
23	Solvothermal-assisted evaporation-induced self-assembly of ordered mesoporous alumina with improved performance. Journal of Colloid and Interface Science, 2018, 529, 432-443.	5.0	10
24	A theoretical study on the structures and electronic and magnetic properties of new boron nitride composite nanosystems by depositing superhalogen Al13on the surface of nanosheets/nanoribbons. Physical Chemistry Chemical Physics, 2018, 20, 15424-15433.	1.3	3
25	A Biomimetic Musselâ€Inspired εâ€Polyâ€ <scp>l</scp> â€lysine Hydrogel with Robust Tissueâ€Anchor and Antiâ€Infection Capacity. Advanced Functional Materials, 2017, 27, 1604894.	7.8	342
26	Covalent surface modification with electron-donating/accepting π-conjugated chains to effectively tune the electronic and magnetic properties of zigzag SiC nanoribbons. Journal of Materials Chemistry C, 2017, 5, 2022-2032.	2.7	7
27	Introducing the triangular BN nanodot or its cooperation with the edge-modification via the electron-donating/withdrawing group to achieve the large first hyperpolarizability in a carbon nanotube system. Physical Chemistry Chemical Physics, 2017, 19, 17834-17844.	1.3	13
28	Adsorbing the 3d-transition metal atoms to effectively modulate the electronic and magnetic behaviors of zigzag SiC nanoribbons. Physical Chemistry Chemical Physics, 2017, 19, 3694-3705.	1.3	9
29	Highly Active, Nonprecious Electrocatalyst Comprising Borophene Subunits for the Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2017, 139, 12370-12373.	6.6	335
30	Enhancing the Hydrogen Activation Reactivity of Nonprecious Metal Substrates via Confined Catalysis Underneath Graphene. Nano Letters, 2016, 16, 6058-6063.	4.5	101
31	Unique Electronic Structure in a Porous Gaâ€In Bimetallic Oxide Nanoâ€Photocatalyst with Atomically Thin Pore Walls. Angewandte Chemie - International Edition, 2016, 55, 11442-11446.	7.2	40
32	Metallic Co ₉ S ₈ nanosheets grown on carbon cloth as efficient binder-free electrocatalysts for the hydrogen evolution reaction in neutral media. Journal of Materials Chemistry A, 2016, 4, 6860-6867.	5.2	265
33	Realizing diverse electronic and magnetic properties in hybrid zigzag BNC nanoribbons via hydrogenation. Physical Chemistry Chemical Physics, 2016, 18, 1326-1340.	1.3	9
34	Coupling Mo ₂ C with Nitrogenâ€Rich Nanocarbon Leads to Efficient Hydrogenâ€Evolution Electrocatalytic Sites. Angewandte Chemie - International Edition, 2015, 54, 10752-10757.	7.2	674
35	A first-principles investigation on the effect of the divacancy defect on the band structures of boron nitride (BN) nanoribbons. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 69, 65-74.	1.3	12
36	Molecular charge transfer via π–π interaction: an effective approach to realize the half-metallicity and spin-gapless-semiconductor in zigzag graphene nanoribbon. RSC Advances, 2015, 5, 53003-53011.	1.7	11

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37	High-Index Faceted Ni ₃ S ₂ Nanosheet Arrays as Highly Active and Ultrastable Electrocatalysts for Water Splitting. Journal of the American Chemical Society, 2015, 137, 14023-14026.	6.6	1,622
38	Adsorbing a PVDF polymer via noncovalent interactions to effectively tune the electronic and magnetic properties of zigzag SiC nanoribbons. Physical Chemistry Chemical Physics, 2015, 17, 24038-24047.	1.3	11
39	Molecular charge transfer by adsorbing TCNQ/TTF molecules via π–π interaction: a simple and effective strategy to modulate the electronic and magnetic behaviors of zigzag SiC nanoribbons. Physical Chemistry Chemical Physics, 2015, 17, 941-950.	1.3	14
40	Constructing a mixed ï€-conjugated bridge to effectively enhance the nonlinear optical response in the Möbius cyclacene-based systems. Physical Chemistry Chemical Physics, 2014, 16, 10933-10942.	1.3	29
41	Dihalogen edge-modification: an effective approach to realize the half-metallicity and metallicity in zigzag silicon carbon nanoribbons. Journal of Materials Chemistry C, 2014, 2, 7836-7850.	2.7	28
42	Introducing the Triangular Defect to Effectively Engineer the Wide Band Gap of Boron Nitride Nanoribbons with Zigzag and Even Armchair Edges. Journal of Physical Chemistry C, 2014, 118, 12880-12889.	1.5	20
43	Doping the Alkali Atom: An Effective Strategy to Improve the Electronic and Nonlinear Optical Properties of the Inorganic Al ₁₂ N ₁₂ Nanocage. Inorganic Chemistry, 2014, 53, 349-358.	1.9	135
44	Constructing (super)alkali–boron-heterofullerene dyads: an effective approach to achieve large first hyperpolarizabilities and high stabilities in M ₃ O–BC ₅₉ (M = Li, Na and K) and K@n-BC ₅₉ (n = 5 and 6). Physical Chemistry Chemical Physics, 2014, 16, 1597-1606.	1.3	64
45	(Super)alkali atoms interacting with the σ electron cloud: a novel interaction mode triggers large nonlinear optical response of M@P4 and M@C3H6 (M=Li, Na, K and Li3O). Journal of Molecular Modeling, 2013, 19, 5601-5610.	0.8	18
46	The donor/acceptor edge-modification: an effective strategy to modulate the electronic and magnetic behaviors of zigzag silicon carbon nanoribbons. Physical Chemistry Chemical Physics, 2013, 15, 18039.	1.3	23
47	An Effective Approach to Achieve a Spin Gapless Semiconductor–Halfâ€Metal–Metal Transition in Zigzag Graphene Nanoribbons: Attaching A Floating Induced Dipole Field via <i>π</i> – <i>π</i> Interactions. Advanced Functional Materials, 2013, 23, 1507-1518.	7.8	37
48	Constructing a mixed π-conjugated bridge: a simple and effective approach to realize a large first hyperpolarizability in carbon nanotube-based systems. Journal of Materials Chemistry C, 2013, 1, 3833.	2.7	36
49	The Effects of the Formation of Stone–Wales Defects on the Electronic and Magnetic Properties of Silicon Carbide Nanoribbons: A Firstâ€Principles Investigation. ChemPhysChem, 2013, 14, 2841-2852.	1.0	37
50	Successive hydrogenation starting from the edge(s): an effective approach to fine-tune the electronic and magnetic behaviors of SiC nanoribbons. Journal of Materials Chemistry, 2012, 22, 24166.	6.7	32
51	Copper nanoclusters: Synthesis, characterization and properties. Science Bulletin, 2012, 57, 41-47.	1.7	113
52	Alkali metal atomâ€aromatic ring: A novel interaction mode realizes large first hyperpolarizabilities of M@AR (M = Li, Na, and K, AR = pyrrole, indole, thiophene, and benzene). Journal of Computational Chemistry, 2011, 32, 2005-2011.	1.5	71
53	Hydrogenation: A Simple Approach To Realize Semiconductorâ^'Half-Metalâ^'Metal Transition in Boron Nitride Nanoribbons. Journal of the American Chemical Society, 2010, 132, 1699-1705.	6.6	277
54	The nitrogen edgeâ€doped effect on the static first hyperpolarizability of the supershort singleâ€walled carbon nanotube. Journal of Computational Chemistry, 2009, 30, 1128-1134.	1.5	46

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55	Investigation on nonlinear optical properties of ladder-structure polydiacetylenes derivatives by using the elongation finite-field method. Chemical Physics Letters, 2009, 474, 175-179.	1.2	25
56	Electronic Structure and Reactivity of Boron Nitride Nanoribbons with Stone-Wales Defects. Journal of Chemical Theory and Computation, 2009, 5, 3088-3095.	2.3	127
57	Structures and Considerable Static First Hyperpolarizabilities:  New Organic Alkalides (M ⁺ @ <i>n</i> ⁶ adz)Mâ€~ ⁻ (M, Mâ€~ = Li, Na, K; <i>n</i> = 2, 3) with Catio Inside and Anion Outside of the Cage Complexants. Journal of Physical Chemistry B, 2008, 112, 1090-1094.	on1.2	109
58	Nonlinear Optical Properties of Alkalides Li+(calix[4]pyrrole)M-(M = Li, Na, and K):Â Alkali Anion Atomic Number Dependence. Journal of the American Chemical Society, 2006, 128, 1072-1073.	6.6	218
59	The Structure and the Large Nonlinear Optical Properties of Li@Calix[4]pyrrole. Journal of the American Chemical Society, 2005, 127, 10977-10981.	6.6	318