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Rank	Title	Author(s)	Journal	Year	Citations
1	Machine-Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene	Mishra, A.; Singh, AK	CHEMISTRY OF MATERIALS	2018	140
2	Tetrahexcarbon: A two-dimensional allotrope of carbon	Ram, B and Mizuseki, H	CARBON	2018	60
3	Simulation Protocol for Prediction of a Solid-Electrolyte Interphase on the Silicon-based Anodes of a Lithium-Ion Battery: ReaxFF Reactive Force Field	Yun, KS; Pai, S.; Han, SS	JOURNAL OF PHYSICAL CHEMISTRY LETTERS	2017	36
4	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study	Mishra, A; Srivastava, P; Singh, AK	JOURNAL OF PHYSICAL CHEMISTRY C	2017	35
5	New carbon allotropes in sp + sp(3) bonding networks consisting of C-8 cubes	Wang, JT; Chen, CF; Kawazoe, Y	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	2018	28

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1 Orthorhombic carbon oC24: A novel topological nodal line semimetal 41 Citations
60 References
Zhang, Z.; Chen, J.; (...); Wang, J.T.
Jul 2018 | CARBON 133, pp.39-43
We identify by ab initio calculations a stable three-dimensional carbon allotrope that constructed by inserting benzene rings into the carbon-carbon bonds in a previously reported oC8 carbon. This new carbon phase has a 24-atom orthorhombic unit cell in Cmmm (D-2H(19)) symmetry and thus termed c... Show more
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2 C-568: A new two-dimensional sp(2)-sp(3) hybridized allotrope of carbon 39 Citations
69 References
Liu, Y.; Kim, D.; (...); Grossman, J.C.
Mar 2020 | CARBON 158, pp.827-835
Using first-principles calculations, we designed a new two-dimensional sp(2)-sp(3) hybridized allotrope of carbon. This allotrope is made up of 5-6-8 carbon rings thus, known as C-568. C-568 is an indirect semiconductor with a band gap of 1.13 eV (HSE06) at Gamma-M symmetric point in the B... Show more
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3 Origins of the Stokes Shift in PbS Quantum Dots: Impact of Polydispersity, Ligands, and Defects 38 Citations
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Liu, Y.; Kim, D.; (...); Grossman, J.C.
Mar 2018 | ACS NANO 12 (3), pp.2838-2845
Understanding the origins of the excessive Stokes shift in the lead chalcogenides family of colloidal quantum dots (CQDs) is of great importance at both the fundamental and applied levels; however, our current understanding is far from satisfactory. Here, utilizing a combination of ab initio com... Show more
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4 Atomistic Sodiation Mechanism of a Phosphorene/Graphene Heterostructure for Sodium-Ion Batteries Determined by First-Principles Calculations 28 Citations
35 References
Lee, H.W.; Jung, H.; (...); Han, S.S.
Sep 13 2018 | JOURNAL OF PHYSICAL CHEMISTRY C 122 (36), pp.20653-20660
Black phosphorus has recently attracted significant attention as an anode material for sodium-ion batteries (SIBs); however, the material suffers from a severe volume change during charge/discharge processes, leading to poor cycle life. To overcome this drawback of black phosphorus, a phosphorene/... Show more
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5 Electron-hole separation in ferroelectric oxides for efficient photovoltaic responses 26 Citations
37 References
Kim, D.; Han, H.; (...); Kim, D.
Jun 26 2018 | PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA

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- 1 A tailored oxide interface creates dense Pt single-atom catalysts with high catalytic activity 76 Citations
Yoo, M; Yu, YS; (...); Kim, HY
Apr 1 2020 | ENERGY & ENVIRONMENTAL SCIENCE 13 (4), pp.1231-1239
Highly reactive dense Pt single-atoms stabilized on an oxide support can resolve a grand challenge in the economic use of Pt in catalysis. The maximized number density of reaction sites provided by dense Pt single-atoms guarantees the improved catalytic performance of Pt combined with high eff... Show more
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- 2 Unlocking the Potential of Nanoparticles Composed of Immiscible Elements for Direct H2O2 Synthesis 21 Citations
Kim, D; Nam, H; (...); Han, SS
Sep 2019 | ACS CATALYSIS 9 (9), pp.8702-8711
Today, multimetallic nanoparticles (NPs) are extensively studied to search for high-performance catalysts. Unfortunately, a huge material space of NPs composed of immiscible elements has been generally disregarded for catalyst development due to the inherent difficulty of alloy synthesis. Herein, for... Show more
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- 3 Understanding the potential band position and e-/h(+) separation lifetime for Z-scheme and type-II heterojunction mechanisms for effective micropollutant mineralization: Comparative experimental and DFT studies 20 Citations
Wong, KT; Kim, SC; (...); Jang, M
Sep 15 2020 | APPLIED CATALYSIS B-ENVIRONMENTAL 273
A new approach to determine the importance of band potential by comparing two different electron charge transfer mechanism, via Z-scheme and type-II heterojunction. Through microwave hydrothermal (MWH) treatment and subsequent thermal polycondensation, the released ammonia gas fr... Show more
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- 4 Medium-range order in amorphous ices revealed by persistent homology 6 Citations
Hong, S and Kim, D
Nov 13 2019 | JOURNAL OF PHYSICS-CONDENSED MATTER 31 (45)
Despite the amorphous nature of glassy water, x-ray or neutron scattering experiments reveal sharp peaks in the structure factor, indicating the existence of medium-range order (MRO) in the system. However the real space origin of the peaks has yet to be disclosed. Herein, we use a combined appro: ... Show more
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- 5 Gdme-SnS: a two-dimensional tin sulfide nanosheet 3 Citations
Ram, B and Mizuseki, H
Oct 28 2020 | JOURNAL OF MATERIALS CHEMISTRY A 8 (40), pp.21219-21226

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- 1 Cooperative carbon capture and steam regeneration with tetraamine-appended metal-organic frameworks 141 Citations 59 References
Kim, E.J.; Siegelman, R.L.; (...); Long, J.R.
Jul 24 2020 | SCIENCE 369 (6502), pp.392-+
Natural gas has become the dominant source of electricity in the United States, and technologies capable of efficiently removing carbon dioxide (CO2) from the flue emissions of natural gas-fired power plants could reduce their carbon intensity. However, given the low partial pressure of CO2 in the ... Show more
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- 2 Self-assembled heterojunction of metal sulfides for improved photocatalysis 31 Citations 47 References
Khan, S.; Choi, H.; (...); Cho, S.H.
Sep 1 2020 | CHEMICAL ENGINEERING JOURNAL 395
Due to its high redox potential, zinc sulfide (ZnS) is considered an excellent semiconductor photocatalyst. However, the rapid recombination rate of the photogenerated electron-hole pairs limits the efficiency of ZnS for photocatalytic reactions. Herein, we suggest a design rule of heterojunction stru ... Show more
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- 3 High Ammonia Uptake of a Metal-Organic Framework Adsorbent in a Wide Pressure Range 27 Citations 45 References
Kim, D.W.; Kang, D.W.; (...); Hong, C.S.
Dec 7 2020 | Nov 2020 (Early Access) | ANGEWANDTE CHEMIE-INTERNATIONAL EDITION 59 (50), pp.22531-22536
Enriched Cited References
Although numerous porous adsorbents have been investigated for NH3 capture applications, these materials often exhibit insufficient NH3 uptake, low NH3 affinity at the ppm level, and poor chemical stability against wet NH3 conditions. The NH3 capture properties of M-2(dobpdc) complexes (M=Mg, ... Show more
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- 4 A recyclable metal-organic framework for ammonia vapour adsorption 17 Citations 26 References
Nguyen, T.N.; Harreschou, I.M.; (...); Stephan, D.W.
Aug 28 2020 | CHEMICAL COMMUNICATIONS 56 (67), pp.9600-9603
Herein, we present a new strategy to design metal-organic frameworks (MOFs) as adsorbents for ammonia (NH3) vapour. The linking ligand is functionalized with a sterically hindered Lewis acidic boron (B) centre, allowing efficient capture of NH3 and easy recycling of the MOF by simply heating a ... Show more
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- 6 Body-centered cubic carbon BC14: An all-sp(3) bonded full-fledged pentadiamond 12 Citations 72 References
Wang, J.T.; Chen, C.F. and Mizuseki, H.
Nov 10 2020 | PHYSICAL REVIEW B 102 (18)
We report on the finding of a hard carbon structure in body centered cubic (I2(1)3) symmetry that possesses an extremely high bulk modulus (386 GPa) and Vickers hardness (60 GPa) comparable to that of c-BN and diamond. This carbon phase has 14 tetrahedral carbon atoms in all sp(3) hybridization. ... Show more

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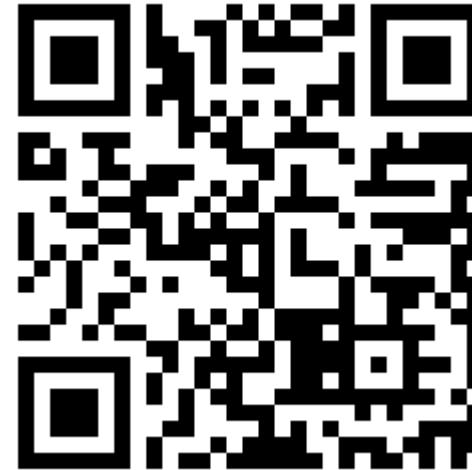
- 1 ZnS/ZnO nanosheets obtained by thermal treatment of ZnS/ethylenediamine as a Z-scheme photocatalyst for H-2 generation and Cr (VI) reduction
Poliukhova, V; Khan, S; (...); Cho, SH
Feb 1 2022 | Nov 2021 (Early Access) | APPLIED SURFACE SCIENCE 575
9 Citations
50 References
In this study, ZnS/ethylenediamine nanosheets were obtained by solvothermal synthesis and modified into composites of ZnS and ZnO by heat treatment. Compared to pure ZnO and ZnS, the ZnS/ZnO composite showed superior photocatalytic activity towards hydrogen evolution from water (5f ... Show more
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- 2 Molecular Dopant-Dependent Charge Transport in Surface-Charge-Transfer-Doped Tungsten Diselenide Field Effect Transistors
Kim, JK; Cho, K; (...); Lee, T
Nov 2021 | Sep 2021 (Early Access) | ADVANCED MATERIALS 33 (44)
7 Citations
54 References
The controllability of carrier density and major carrier type of transition metal dichalcogenides(TMDCs) is critical for electronic and optoelectronic device applications. To utilize doping in TMDC devices, it is important to understand the role of dopants in charge transport properties of TMDCs. Here, th ... Show more
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- 3 Atomistic origin of compositional pulling effect in wurtzite (B, Al, In)(x)Ga1-xN: A first-principles study
Mizuseki, H; Gueriba, JS; (...); Ohkawa, K
Jul 21 2021 | JOURNAL OF APPLIED PHYSICS 130 (3)
3 Citations
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Some fluctuations in composition are commonly observed in epitaxial-grown III-V multinary alloys. These fluctuations are attributed to compositional pulling effects, and an insight into their atomistic origin is necessary to improve current epitaxial growth techniques. In addition, the crystallin ... Show more
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- 4 An assessment of density functionals for predicting CO2 adsorption in diamine-functionalized metal-organic frameworks
Lee, JH; Hyldgaard, P and Neaton, JB
Apr 21 2022 | JOURNAL OF CHEMICAL PHYSICS 156 (15)
2 Citations
95 References
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Diamine-functionalized M-2(dobpdc) (M = Mg, Mn, Fe, Co, Zn) metal-organic frameworks (MOFs) are among a growing class of crystalline solids currently being intensively investigated for carbon capture as they exhibit a novel cooperative and selective CO2 adsorption mechanism and a step-shaped isot ... Show more

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