Wan-Sheng Su

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Relationship between surface dipole, work function and charge transfer:â€,â€,Some exceptions to an established rule. Physical Review B, 2003, 68, .	1.1	344
2	Work function of single-walled and multiwalled carbon nanotubes: First-principles study. Physical Review B, 2007, 76, .	1.1	147
3	Electronic and optical properties of novel carbon allotropes. Carbon, 2016, 101, 77-85.	5.4	98
4	A new carbon allotrope: Penta-graphene as a metal-free catalyst for CO oxidation. Carbon, 2017, 114, 465-472.	5.4	91
5	Strain driven topological phase transitions in atomically thin films of group IV and V elements in the honeycomb structures. New Journal of Physics, 2014, 16, 105018.	1.2	58
6	A first-principles study of the electronic structure and mechanical and optical properties of CaAlSiN ₃ . Physical Chemistry Chemical Physics, 2015, 17, 15065-15070.	1.3	33
7	Electronic and optical properties of single-walled carbon nanotubes under a uniform transverse electric field: A first-principles study. Physical Review B, 2009, 79, .	1.1	32
8	Work function of small radius carbon nanotubes and their bundles. Applied Physics Letters, 2007, 90, 163103.	1.5	24
9	Structural and electronic properties of hydrogen adsorptions on BC ₃ sheet and graphene: a comparative study. Nanotechnology, 2011, 22, 135703.	1.3	24
10	Electronic and optical properties of hydrogen-terminated biphenylene nanoribbons: a first-principles study. Physical Chemistry Chemical Physics, 2021, 24, 357-365.	1.3	23
11	Bergman-type medium range order in amorphous Zr77Rh23 alloy studied by ab initio molecular dynamics simulations. Journal of Alloys and Compounds, 2019, 790, 675-682.	2.8	22
12	Electronic structures and work functions of BC3 nanotubes: A first-principle study. Journal of Applied Physics, 2011, 110, .	1.1	20
13	Novel penta-graphene nanotubes: strain-induced structural and semiconductor–metal transitions. Nanoscale, 2017, 9, 19310-19317.	2.8	18
14	A first-principles study on the electromechanical effect of graphene nanoribbon. Computer Physics Communications, 2011, 182, 99-102.	3.0	17
15	Quantum confinement effect in armchair graphene nanoribbons: Effect of strain on band gap modulation studied using first-principles calculations. Physical Review B, 2014, 90, .	1.1	15
16	Tunable magnetic states on the zigzag edges of hydrogenated and halogenated group-IV nanoribbons. Scientific Reports, 2016, 6, 39083.	1.6	15
17	A first-principles study of the electrically tunable band gap in few-layer penta-graphene. Physical Chemistry Chemical Physics, 2018, 20, 18110-18116.	1.3	14
18	The fracture behaviors of monolayer phosphorene with grain boundaries under tension: a molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 20562-20570.	1.3	13

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19	Electric Field-Tunable Structural Phase Transitions in Monolayer Tellurium. ACS Omega, 2020, 5, 18213-18217.	1.6	11
20	The screening effect on field enhancement factor of the finite-length small radius single-walled carbon nanotubes. Journal of Applied Physics, 2009, 106, 014301.	1.1	10
21	Electronic structure and optical properties of boron suboxide B6O system: First-principles investigations. Solid State Communications, 2016, 244, 12-16.	0.9	10
22	Theoretical investigation of methane oxidation reaction over a novel metal-free catalyst biphenylene network. Diamond and Related Materials, 2022, 124, 108897.	1.8	10
23	Competitive diamondâ€like and endohedral fullerene structures of Si ₇₀ . Journal of Computational Chemistry, 2011, 32, 1271-1278.	1.5	9
24	Si ₇₈ double cage structure and special optical properties. Physical Chemistry Chemical Physics, 2015, 17, 27734-27741.	1.3	9
25	Si-centered capped trigonal prism ordering in liquid Pd ₈₂ Si ₁₈ alloy study by first-principles calculations. RSC Advances, 2017, 7, 18093-18098.	1.7	9
26	Strain effects on the band gap and work function of zigzag single-walled carbon nanotubes and graphene: A comparative study. Computer Physics Communications, 2014, 185, 1422-1428.	3.0	8
27	Structural, electronic, and optical properties of α-Te tubular nanostructures: A first-principles study. APL Materials, 2019, 7, .	2.2	8
28	Structural and electronic properties of graphene nanotube–nanoribbon hybrids. Physical Chemistry Chemical Physics, 2011, 13, 3925.	1.3	7
29	Electronic and optical properties of bundled single-walled carbon nanotubes investigated by the first-principles method. Computer Physics Communications, 2013, 184, 1077-1085.	3.0	7
30	Investigation into the mechanical properties of single-walled carbon nanotube heterojunctions. Physical Chemistry Chemical Physics, 2013, 15, 11579.	1.3	6
31	Electronic and structural properties of carbon nanotubes modulated by external strain. Journal of Applied Physics, 2013, 113, .	1.1	6
32	Screening effects on the field enhancement factor of zigzag graphene nanoribbon arrays: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 14627-14634.	1.3	6
33	Investigation of electronic property modulation driven by strain in monolayer tellurium. Chinese Journal of Physics, 2019, 62, 172-178.	2.0	6
34	A first-principles study of strain tuned optical properties in monolayer tellurium. RSC Advances, 2019, 9, 41703-41708.	1.7	6
35	Nanomeasurements of electronic and mechanical properties of fullerene embedded Si(111) surfaces. Applied Physics Letters, 2010, 97, 061908.	1.5	5
36	Atomic structure and mechanical properties of BC2N superlattice. Diamond and Related Materials, 2010, 19, 1341-1347.	1.8	5

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37	Characteristics of Si(111) surface with embedded C84 molecules. RSC Advances, 2013, 3, 9234.	1.7	5
38	Magnetic evolution and anomalous Wilson transition in diagonal phosphorene nanoribbons driven by strain. Nanotechnology, 2015, 26, 295402.	1.3	5
39	Structural and optical properties of Ge60Te40: experimental and theoretical verification. Journal Physics D: Applied Physics, 2016, 49, 155105.	1.3	5
40	Luminescence mechanism in hydrogenated silicon quantum dots with a single oxygen ligand. Nanoscale Advances, 2021, 3, 2245-2251.	2.2	5
41	A first-principles study of electronic and optical properties of the tetragonal phase of monolayer ZnS modulated by biaxial strain. RSC Advances, 2022, 12, 6166-6173.	1.7	5
42	Influence of strain on the hexagonal motifs of the Ir(100) surface reconstructions: A first-principles study. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2010, 28, 1366-1370.	0.9	4
43	Low-energy electronic structures of nanotube–nanoribbon hybrid systems. Computer Physics Communications, 2011, 182, 68-70.	3.0	4
44	Target Molecular Simulations of RecA Family Protein Filaments. International Journal of Molecular Sciences, 2012, 13, 7138-7148.	1.8	4
45	Effect of body defect on mechanical behaviors of Cu nanowire under tension: a molecular dynamics investigation. Journal of Materials Science, 2017, 52, 13237-13246.	1.7	4
46	Temperature dependence of structural, dynamical, and electronic properties of amorphous Bi ₂ Te ₃ : an ab initio study. New Journal of Physics, 2019, 21, 093062.	1.2	4
47	Low-energy electronic properties of finite double-walled carbon nanotubes under external fields. Physica E: Low-Dimensional Systems and Nanostructures, 2009, 41, 1226-1231.	1.3	3
48	Tuning the electronic properties of monolayer graphene by the periodic aligned graphene nanoribbons. Synthetic Metals, 2011, 161, 489-495.	2.1	3
49	Plasmonic photocatalytic reactions enhanced by hot electrons in a one-dimensional quantum well. AIP Advances, 2015, 5, 117224.	0.6	3
50	Optical Properties and Local Structure Evolution during Crystallization of Ga16Sb84 Alloy. Scientific Reports, 2018, 8, 9605.	1.6	3
51	Low-energy Landau levels of Bernal zigzag graphene ribbons. Journal of Applied Physics, 2009, 106, .	1.1	2
52	Influence of oriented topological defects on the mechanical properties of carbon nanotube heterojunctions. Journal of Applied Physics, 2013, 114, 144306.	1.1	2
53	A first-principles study of structural, electronic and optical properties of α-Te tubular nanostructures modulated by uniaxial strain. New Journal of Physics, 2022, 24, 053037.	1.2	2
54	A new direct band gap Si–Ge allotrope with advanced electronic and optical properties. Physical Chemistry Chemical Physics, 2022, 24, 16310-16316.	1.3	2

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55	Electronic properties of bilayer AA-stacked zigzag nanographene ribbons. Diamond and Related Materials, 2011, 20, 505-508.	1.8	1
56	Investigation into the formation of 13-6 helical multi-shell gold nanowires. Computational Materials Science, 2014, 82, 226-230.	1.4	1
57	Using a functional C ₈₄ monolayer to improve the mechanical properties and alter substrate deformation. RSC Advances, 2015, 5, 47498-47505.	1.7	1
58	Examining the Trend of Taiwan Primary and High School Scientific Exhibition by Using Text Mining Technique. , 2017, , .		1
59	Diffusion of the vacancy defect leading to the formation of multi-shell structures in the nanowire and nanobridge. Journal of Applied Physics, 2012, 112, 114301.	1.1	Ο
60	Effects of Cs adsorption on the field emission characteristics of closed single-walled carbon nanotubes. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2013, 31, 021802.	0.6	0
61	Theoretical study on nanostructural modifications of the Si(111) surface. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950005.	1.8	0
62	Properties of Si nanostructural modification on Si (111) surface. Chinese Journal of Physics, 2020, 67, 69-78.	2.0	0