

# Chunmei Tang

## List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Remarkable-cycle-performance $\hat{I}^2$ -bismuthene/graphene heterostructure anode for Li-ion battery. Chinese Chemical Letters, 2022, 33, 3802-3808.	9.0	8
2	Theoretically identifying the electrocatalytic activity and mechanism of Zn doped 2D h-BN for nitrate reduction to $\text{NH}_3$ . Chemical Communications, 2022, 58, 7156-7159.	4.1	7
3	The first-principles study on the performance of the graphene/WS <sub>2</sub> heterostructure as an anode material of Li-ion battery. Journal of Alloys and Compounds, 2021, 855, 157432.	5.5	30
4	Research on metallic chalcogen-functionalized monolayer-puckered V <sub>2</sub> CX <sub>2</sub> (X) Tj ETQq0 0.0 rgBT /Overlock 10 4672-4681.	5.9	8
5	Remarkable-cycling-performance anode for Li-ion battery: The bilayer $\hat{I}^2$ -bismuthene. Electrochimica Acta, 2021, 388, 138641.	5.2	7
6	Promising anode material BN/VS <sub>2</sub> heterostructure for the Li-ion battery: The first-principles study. Applied Surface Science, 2021, 564, 150468.	6.1	23
7	An effective method to screen carbon (boron, nitrogen) based two-dimensional hydrogen storage materials. International Journal of Hydrogen Energy, 2020, 45, 25054-25064.	7.1	13
8	The First-Principles Prediction of Two Dimensional Monolayer Puckered WCAZ <sub>2</sub> as the Anode Material of Li-ion Batteries. Materials Today Communications, 2020, 25, 101587.	1.9	1
9	Synthesis of nickel selenide thin films for high performance all-solid-state asymmetric supercapacitors. Chinese Chemical Letters, 2020, 31, 2275-2279.	9.0	18
10	Hydrogen trapping efficiency of Li decorated porous boron fullerene B <sub>38</sub> : The first-principles study. International Journal of Hydrogen Energy, 2020, 45, 21646-21654.	7.1	11
11	Multiple Regulation over Growth Direction, Band Structure, and Dimension of Monolayer WS <sub>2</sub> by a Quartz Substrate. Chemistry of Materials, 2020, 32, 2508-2517.	6.7	21
12	How a trapeziform flake of monolayer WS <sub>2</sub> formed on SiO <sub>2</sub> (110)? A first-principle study. Applied Surface Science, 2020, 517, 145864.	6.1	2
13	The good performance of bilayer $\hat{I}^2$ -antimonene as an anode material for the Li-ion battery study. Applied Surface Science, 2019, 495, 143549.	6.1	17
14	The first-principle study on the performance of biaxial strained graphdiyne as the Li-ion battery anode. Applied Surface Science, 2019, 497, 143723.	6.1	24
15	Theoretical investigating of graphene/antimonene heterostructure as a promising high cycle capability anodes for fast-charging lithium ion batteries. Applied Surface Science, 2019, 491, 451-459.	6.1	33
16	Oil boundary approach for sublimation enabled camphor mediated graphene transfer. Journal of Colloid and Interface Science, 2019, 546, 11-19.	9.4	13
17	Density functional calculations of efficient H <sub>2</sub> separation from impurity gases (H) Tj ETQq1 1 0.784314 rgBT /Overlock 10 bilayer g-C <sub>3</sub> N. Chinese Physics B, 2019, 28, 048102.	1.4	14
18	A New Effective Approach to Prevent the Degradation of Black Phosphorus: The Scandium Transition Metal Doping. Journal of Physical Chemistry C, 2018, 122, 9654-9662.	3.1	20

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19	Strain-Enhanced Li Storage and Diffusion on the Graphyne as the Anode Material in the Li-Ion Battery. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22838-22848.	3.1	58
20	Most effective way to improve the hydrogen storage abilities of Na-decorated BN sheets: applying external biaxial strain and an electric field. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5570-5578.	2.8	23
21	Enhanced optical spin current injection in the hexagonal lattice with intrinsic and Rashba spin-orbit interactions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 1197-1201.	2.1	5
22	The Peculiar Role of the Au <sub>3</sub> Unit in Au <sub>m</sub> Clusters: $\pi$ -Aromaticity of the Au <sub>5</sub> Zn <sup>+</sup> Ion. <i>Inorganic Chemistry</i> , 2017, 56, 5793-5803.	4.0	27
23	Dynamical energy equipartition of the Toda model with additional on-site potentials. <i>Chinese Physics B</i> , 2017, 26, 100505.	1.4	6
24	Vertically-aligned Mn(OH) <sub>2</sub> nanosheet films for flexible all-solid-state electrochemical supercapacitors. <i>Journal of Materials Science: Materials in Electronics</i> , 2017, 28, 17533-17540.	2.2	24
25	The reversible hydrogen storage abilities of metal Na (Li, K, Ca, Mg, Sc, Ti, Y) decorated all-boron cage B <sub>28</sub> . <i>International Journal of Hydrogen Energy</i> , 2017, 42, 16611-16619.	7.1	60
26	The Magnetic Transition of Tcn (n=1, 2) Induced by the Reaction with Cl and BO <sub>2</sub> . <i>Journal of Cluster Science</i> , 2017, 28, 905-915.	3.3	0
27	The hydrogen storage capacity of Sc atoms decorated porous boron fullerene B <sub>40</sub> : A DFT study. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 16992-16999.	7.1	74
28	The hydrogen storage properties of Na decorated small boron cluster B <sub>6</sub> Na <sub>8</sub> . <i>Chemical Physics Letters</i> , 2016, 661, 161-167.	2.6	14
29	Electric field induced enhancement of hydrogen storage capacity for Li atom decorated graphene with Stone-Wales defects. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 10776-10785.	7.1	73
30	How will the benzyne group $\text{C}_6\text{H}_4$ affect the structure, electronic and optical properties of M <sub>3</sub> N@C <sub>80</sub> (M = Sc, Y)? <i>Computational and Theoretical Chemistry</i> , 2016, 1084, 17-24.	2.5	7
31	The hydrogen storage properties of the Ti decorated benzene-Ti-graphene sandwich-type structures. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 1035-1043.	7.1	21
32	The determination of serum cholesterol concentration with improved differential evolution algorithm based on ultraviolet-visible absorption spectrum. , 2016, , .		0
33	Numerical and Experimental Investigation on Electromagnetic Attenuation by Semi-Ellipsoidal Shaped Plasma. <i>Plasma Science and Technology</i> , 2015, 17, 869-875.	1.5	15
34	Transition metal Ti coated porous fullerene C <sub>24</sub> B <sub>24</sub> : Potential material for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 16271-16277.	7.1	51
35	The properties of hydrogenated derivatives of the alkali atom coated clusters C <sub>6</sub> M <sub>6</sub> (M=Li, Na): A density functional study. <i>Computational and Theoretical Chemistry</i> , 2015, 1071, 46-52.	2.5	2
36	The study of the hydrogen storage capacity of the Ti atoms coated Si@Ga <sub>12</sub> clusters. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 16278-16287.	7.1	1

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37	Geometric Structure, Electronic Property, and Hydrogen Storage Capacity of the Sc Atoms Decorated Expanded Sandwich Type Structure Graphene-Sc-graphene. <i>Acta Chimica Sinica</i> , 2015, 73, 1189.	1.4	2
38	Stabilities, aromaticity, infrared spectra, and optical properties of exohedral fullerene derivatives C <sub>76</sub> X <sub>18</sub> (X = H, F, Cl, and Br). <i>European Physical Journal D</i> , 2014, 68, 1.	1.3	2
39	Doping the transition metal atom Fe, Co, Ni into C <sub>48</sub> B <sub>12</sub> fullerene for enhancing H <sub>2</sub> capture: A theoretical study. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 12741-12748.	7.1	24
40	The density functional studies of the doped gold cages Au <sub>17</sub> M (M=Cu, Ag, Li, Na, K). <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 62-66.	2.5	5
41	Endohedrally doping the gold cage with a trivalent atom B, Al, Ga, and In: Density functional studies. <i>Computational and Theoretical Chemistry</i> , 2013, 1018, 1-5.	2.5	5
42	STRUCTURAL, ELECTRONIC, MAGNETIC, AND OPTICAL PROPERTIES OF 3d TRANSITION METAL ENDOHEDRAL M@Ge <sub>12</sub> H <sub>12</sub> (M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, I, Pt, Au, Hg, Pb, Bi, Po, At, Rn) CLUSTERS. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350063.	2.5	5
43	The high-capacity hydrogen storage abilities of the Ti atoms coated Si@Al <sub>12</sub> clusters. <i>Chemical Physics Letters</i> , 2013, 586, 116-120.	2.6	2
44	Density functional studies of magic clusters Ga <sub>13</sub> M (M=Li, Na, K, and Rb). <i>Computational and Theoretical Chemistry</i> , 2013, 1014, 8-12.	2.5	2
45	Density functional study on the electronic properties, polarizabilities, NICS values, and absorption spectra of fluorinated fullerene derivative C <sub>60</sub> F <sub>17</sub> CF <sub>3</sub> . <i>Computational and Theoretical Chemistry</i> , 2012, 991, 154-160.	2.5	9
46	Nonclassical fullerene C <sub>22</sub> H <sub>22</sub> doped with transition metal atoms (ScNi): Density functional calculations. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 225-230.	2.5	0
47	Probing the geometric, optical, and magnetic properties of 3d transition-metal endohedral Ge <sub>12</sub> M (M=Sc-Ni) clusters. <i>Computational and Theoretical Chemistry</i> , 2011, 969, 56-60.	2.5	34
48	Density Functional Study of Two Seven-Membered Unconventional Fullerenes C <sub>58</sub> F <sub>17</sub> CF <sub>3</sub> and C <sub>58</sub> F <sub>18</sub> . <i>Chinese Journal of Chemistry</i> , 2010, 28, 1355-1358.	4.9	5
49	Density functional energetics and frontier orbitals analysis for the derivatives of the nonclassical triplet-pentagon-fusion fullerene C <sub>64</sub> X (X=Si and Ge). <i>Computational and Theoretical Chemistry</i> , 2010, 950, 36-40.	1.5	6
50	The evolutions of the structure stability, vibrational frequency, frontier orbital, and electronegativity of the unconventional exohedral fullerenes C <sub>64</sub> X <sub>4</sub> (X=H, F, Cl, Br, and I): A density functional study. <i>Computational and Theoretical Chemistry</i> , 2009, 909, 43-48.	1.5	23
51	How will the dichlophenyl group affect the geometric structure, electronic properties, and static linear polarizability of La@C <sub>72</sub> ?. <i>Computational and Theoretical Chemistry</i> , 2009, 894, 112-116.	1.5	14
52	The geometric and magnetic properties of the endohedral plumbaspherene M@Pb <sub>12</sub> clusters (M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, I, Pt, Au, Hg, Pb, Bi, Po, At, Rn). <i>Journal of Theoretical and Computational Chemistry</i> , 2009, 8, 1-5.	2.6	26
53	The density functional calculations on the structural stability, electronic properties, and static linear polarizability of the endohedral metallofullerene Ba@C <sub>74</sub> . <i>Computational and Theoretical Chemistry</i> , 2008, 867, 111-115.	1.5	19
54	The geometric, optical, and magnetic properties of the endohedral stannaspherenes M@Sn <sub>12</sub> (M=Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, I, Pt, Au, Hg, Pb, Bi, Po, At, Rn). <i>Journal of Theoretical and Computational Chemistry</i> , 2008, 7, 1-5.	3.0	30

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55	A theoretical study of the TiC <sub>5</sub> cluster. Journal of Chemical Physics, 2008, 128, 064314.	3.0	4
56	Influence of a dichlophenyl group on the geometric structure, electronic properties, and static linear polarizability of La@C <sub>74</sub> . Physical Review A, 2007, 76, .	2.5	16
57	Geometric and electronic properties of endohedral Si@C <sub>74</sub> . Journal of Chemical Physics, 2006, 125, 104307.	3.0	16
58	Effective High-throughput Screening of Two-Dimensional Layered Materials for Potential Lithium-ion battery Anodes. Dalton Transactions, 0, , .	3.3	0