Frantisek Karlicky

List of Publications by Year in descending order

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45 papers

2,838 citations

279798 23 h-index 233421 45 g-index

45 all docs

45 does citations

45 times ranked

4173 citing authors

#	Article	IF	CITATIONS
1	DFTB investigations of the electronic and magnetic properties of fluorographene with vacancies and with adsorbed chemical groups. Physical Chemistry Chemical Physics, 2022, 24, 3312-3321.	2.8	4
2	Optical gaps and excitons in semiconducting transition metal carbides (MXenes). Journal of Materials Chemistry C, 2022, 10, 3919-3928.	5.5	13
3	Iron Nitride Nanoparticles for Enhanced Reductive Dechlorination of Trichloroethylene. Environmental Science & Environmental S	10.0	30
4	Giant Linear and Nonlinear Excitonic Responses in an Atomically Thin Indirect Semiconductor Nitrogen Phosphide. Journal of Physical Chemistry C, 2021, 125, 12738-12757.	3.1	12
5	Lattice dynamics in the conformational environment of multilayered hexagonal boron nitride (h-BN) results in peculiar infrared optical responses. Physical Chemistry Chemical Physics, 2021, 23, 7247-7260.	2.8	3
6	Fundamental gap of fluorographene by many-body GW and fixed-node diffusion Monte Carlo methods. Journal of Chemical Physics, 2020, 153, 184706.	3.0	17
7	Optical Gaps and Excitonic Properties of 2D Materials by Hybrid Time-Dependent Density Functional Theory: Evidences for Monolayers and Prospects for van der Waals Heterostructures. Journal of Chemical Theory and Computation, 2020, 16 , 5876 - 5883 .	5.3	21
8	A theoretical study of adsorption on iron sulfides towards nanoparticle modeling. Physical Chemistry Chemical Physics, 2020, 22, 23258-23267.	2.8	9
9	Highly Ordered Nâ€Doped Carbon Dots Photosensitizer on Metal–Organic Frameworkâ€Decorated ZnO Nanotubes for Improved Photoelectrochemical Water Splitting. Small, 2019, 15, e1902771.	10.0	66
10	Accurate many-body calculation of electronic and optical band gap of bulk hexagonal boron nitride. Physical Chemistry Chemical Physics, 2019, 21, 3999-4005.	2.8	35
11	Sbâ€Doped SnO ₂ Nanorods Underlayer Effect to the αâ€Fe ₂ O ₃ Nanorods Sheathed with TiO ₂ for Enhanced Photoelectrochemical Water Splitting. Small, 2018, 14, e1703860.	10.0	69
12	Fluorographane C2FH: Stable and wide band gap insulator with huge excitonic effect. Carbon, 2018, 135, 134-144. Photoabsorption spectra of small symplement xmlns/mml="http://www.w3.org/1998/Math/Math/M."	10.3	27
13	altimg="si33.gif" overflow="scroll"> <mml:mrow><mml:mrow><mml:mtext>He</mml:mtext></mml:mrow><mm< td=""><td>l:mrow><r< td=""><td>nml:mi>N</td></r<></td></mm<></mml:mrow>	l:mrow> <r< td=""><td>nml:mi>N</td></r<>	nml:mi>N

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19	Fluorinated graphenes as advanced biosensors – effect of fluorine coverage on electron transfer properties and adsorption of biomolecules. Nanoscale, 2016, 8, 12134-12142.	5.6	60
20	Modelling of graphene functionalization. Physical Chemistry Chemical Physics, 2016, 18, 6351-6372.	2.8	190
21	Thiofluorographene–Hydrophilic Graphene Derivative with Semiconducting and Genosensing Properties. Advanced Materials, 2015, 27, 2305-2310.	21.0	84
22	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. Journal of Physical Chemistry Letters, 2015, 6, 1430-1434.	4.6	90
23	Graphene: Thiofluorographene–Hydrophilic Graphene Derivative with Semiconducting and Genosensing Properties (Adv. Mater. 14/2015). Advanced Materials, 2015, 27, 2407-2407.	21.0	4
24	The surface and structural properties of graphite fluoride. Carbon, 2015, 94, 804-809.	10.3	53
25	Interplay between Ethanol Adsorption to High-Energy Sites and Clustering on Graphene and Graphite Alters the Measured Isosteric Adsorption Enthalpies. Journal of Physical Chemistry C, 2015, 119, 20535-20543.	3.1	31
26	Quantum modelling of hydrogen chemisorption on graphene and graphite. Journal of Chemical Physics, 2014, 140, 124702.	3.0	18
27	Band gaps and optical spectra from single†and doubleâ€layer fluorographene to graphite fluoride: manyâ€body effects and excitonic states. Annalen Der Physik, 2014, 526, 408-414.	2.4	49
28	Anaerobic Reaction of Nanoscale Zerovalent Iron with Water: Mechanism and Kinetics. Journal of Physical Chemistry C, 2014, 118, 13817-13825.	3.1	114
29	Challenges in the theoretical description of nanoparticle reactivity: Nano zeroâ€valent iron. International Journal of Quantum Chemistry, 2014, 114, 987-992.	2.0	14
30	Band Gaps and Optical Spectra of Chlorographene, Fluorographene and Graphane from G _O W _O , GW _O and GW Calculations on Top of PBE and HSE06 Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 4155-4164.	5. 3	142
31	Adsorption of Small Organic Molecules on Graphene. Journal of the American Chemical Society, 2013, 135, 6372-6377.	13.7	407
32	Halogenated Graphenes: Rapidly Growing Family of Graphene Derivatives. ACS Nano, 2013, 7, 6434-6464.	14.6	349
33	Random Phase Approximation in Surface Chemistry: Water Splitting on Iron. Journal of Chemical Theory and Computation, 2013, 9, 3670-3676.	5.3	39
34	Photoabsorption spectrum of helium trimer cation—Theoretical modeling. Journal of Chemical Physics, 2013, 139, 204310.	3.0	5
35	Ligand effects on single-electron transfer of isolated iron atoms in the gaseous complexes $[(OC)mFe(OH2)n]+(m, n=0ae^2, m+n=1, 2)$. International Journal of Mass Spectrometry, 2012, 330-332, 95-99.	1.5	4
36	Band gaps and structural properties of graphene halides and their derivates: A hybrid functional study with localized orbital basis sets. Journal of Chemical Physics, 2012, 137, 034709.	3.0	101

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#	Article	IF	CITATIONS
37	First Step in the Reaction of Zerovalent Iron with Water. Journal of Chemical Theory and Computation, 2011, 7, 2876-2885.	5.3	23
38	Theoretical modeling of ionization energies of argon clusters: Nuclear delocalization effects. Journal of Chemical Physics, 2011, 134, 224310.	3.0	8
39	Vibrational spectrum of Ar3+ and relative importance of linear and perpendicular isomers in its photodissociation. Journal of Chemical Physics, 2011, 134, 084305.	3.0	6
40	Graphene Fluoride: A Stable Stoichiometric Graphene Derivative and its Chemical Conversion to Graphene. Small, 2010, 6, 2885-2891.	10.0	386
41	Structures and energetics of helium cluster cations: Equilibrium geometries revisited through the genetic algorithm approach. Journal of Chemical Physics, 2010, 133, 164314.	3.0	16
42	Modeling of HeN+ clusters. II. Calculation of He3+ vibrational spectrum. Journal of Chemical Physics, 2008, 128, 124303.	3.0	9
43	Calculation of argon trimer rovibrational spectrum. Journal of Chemical Physics, 2007, 126, 174305.	3.0	27
44	Third Virial Coefficients of Argon from First Principles. Journal of Physical Chemistry C, 2007, 111, 15565-15568.	3.1	21
45	Modeling of <mml:math altimg="si1/.gif" overflow="scroll" xmins:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>He</mml:mtext></mml:mrow><mml <="" <mml:math="" ab="" altimg="si18.gif" analytical="" and="" clusters="" energy="" excited="" for="" ground="" i.="" initio="" lowest="" of="" potential="" state="" states="" surfaces="" td="" the="" two="" xmlns:mml="http://www.w3.org/1998/Math/MathML"><td>:mrow><n 1.9</n </td><td>nml:mi>N5</td></mml></mml:msubsup></mml:mrow></mml:math>	:mrow> <n 1.9</n 	nml:mi>N5