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 docs citations	45 times ranked	4173 citing authors

#	Article	IF	Citations
1	Adsorption of Small Organic Molecules on Graphene. Journal of the American Chemical Society, 2013, 135, 6372-6377.	13.7	407
2	Graphene Fluoride: A Stable Stoichiometric Graphene Derivative and its Chemical Conversion to Graphene. Small, 2010, 6, 2885-2891.	10.0	386
3	Halogenated Graphenes: Rapidly Growing Family of Graphene Derivatives. ACS Nano, 2013, 7, 6434-6464.	14.6	349
4	Modelling of graphene functionalization. Physical Chemistry Chemical Physics, 2016, 18, 6351-6372.	2.8	190
5	Band Gaps and Optical Spectra of Chlorographene, Fluorographene and Graphane from G₀W₀, GW₀ and GW Calculations on Top of PBE and HSE06 Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 4155-4164.	5.3	142
6	Anaerobic Reaction of Nanoscale Zerovalent Iron with Water: Mechanism and Kinetics. Journal of Physical Chemistry C, 2014, 118, 13817-13825.	3.1	114
7	Room temperature organic magnets derived from sp3 functionalized graphene. Nature Communications, 2017, 8, 14525.	12.8	112
8	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
9	Î±-Fe₂O₃/TiO₂3D hierarchical nanostructures for enhanced photoelectrochemical water splitting. Nanoscale, 2017, 9, 134-142.	5.6	97
10	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. Journal of Physical Chemistry Letters, 2015, 6, 1430-1434.	4.6	90
11	Thiofluorographeneâ€“Hydrophilic Graphene Derivative with Semiconducting and Genosensing Properties. Advanced Materials, 2015, 27, 2305-2310.	21.0	84
12	Sbâ€Doped SnO₂ Nanorods Underlayer Effect to the Î±â€Fe₂O₃ Nanorods Sheathed with TiO₂ for Enhanced Photoelectrochemical Water Splitting. Small, 2018, 14, e1703860.	10.0	69
13	Highly Ordered Nâ€Doped Carbon Dots Photosensitizer on Metalâ€“Organic Frameworkâ€Decorated ZnO Nanotubes for Improved Photoelectrochemical Water Splitting. Small, 2019, 15, e1902771.	10.0	66
14	Fluorinated graphenes as advanced biosensors â€“ effect of fluorine coverage on electron transfer properties and adsorption of biomolecules. Nanoscale, 2016, 8, 12134-12142.	5.6	60
15	The surface and structural properties of graphite fluoride. Carbon, 2015, 94, 804-809.	10.3	53
16	Band gaps and optical spectra from singleâ€•and doubleâ€layer fluorographene to graphite fluoride: manyâ€body effects and excitonic states. Annalen Der Physik, 2014, 526, 408-414.	2.4	49
17	Adsorption of Organic Molecules to van der Waals Materials: Comparison of Fluorographene and Fluorographite with Graphene and Graphite. Journal of Chemical Theory and Computation, 2017, 13, 1328-1340.	5.3	47
18	Random Phase Approximation in Surface Chemistry: Water Splitting on Iron. Journal of Chemical Theory and Computation, 2013, 9, 3670-3676.	5.3	39

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19	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
20	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
21	Iron Nitride Nanoparticles for Enhanced Reductive Dechlorination of Trichloroethylene. Environmental Science & Technology, 2022, 56, 4425-4436.	10.0	30
22	Calculation of argon trimer rovibrational spectrum. Journal of Chemical Physics, 2007, 126, 174305.	3.0	27
23	Fluorographane C2FH: Stable and wide band gap insulator with huge excitonic effect. Carbon, 2018, 135, 134-144.	10.3	27
24	First Step in the Reaction of Zerovalent Iron with Water. Journal of Chemical Theory and Computation, 2011, 7, 2876-2885.	5.3	23
25	Third Virial Coefficients of Argon from First Principles. Journal of Physical Chemistry C, 2007, 111, 15565-15568.	3.1	21
26	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
27	Quantum modelling of hydrogen chemisorption on graphene and graphite. Journal of Chemical Physics, 2014, 140, 124702.	3.0	18
28	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
29	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
30	Challenges in the theoretical description of nanoparticle reactivity: Nano zeroâ€valent iron. International Journal of Quantum Chemistry, 2014, 114, 987-992.	2.0	14
31	Transformations of ferrates(<scp>iv</scp>,<scp>v</scp>,<scp>vi</scp>) in liquids: MÃ¶ssbauer spectroscopy of frozen solutions. Physical Chemistry Chemical Physics, 2018, 20, 30247-30256.	2.8	13
32	Optical gaps and excitons in semiconducting transition metal carbides (MXenes). Journal of Materials Chemistry C, 2022, 10, 3919-3928.	5.5	13
33	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
34	Modeling of HeN+ clusters. II. Calculation of He3+ vibrational spectrum. Journal of Chemical Physics, 2008, 128, 124303.	3.0	9
35	A theoretical study of adsorption on iron sulfides towards nanoparticle modeling. Physical Chemistry Chemical Physics, 2020, 22, 23258-23267.	2.8	9
36	Theoretical modeling of ionization energies of argon clusters: Nuclear delocalization effects. Journal of Chemical Physics, 2011, 134, 224310.	3.0	8

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37	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
38	Modeling of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si17.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>He</mml:mtext></mml:mrow><mml:mrow><mml:mi>N</mml:mi></mr clusters I. Ab initio and analytical potential energy surfaces for the ground state and two lowest excited states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si18.gif" overflow="scroll"><mml:mrow><mm. Chemical Physics, 2007, 342, 64-70.	1.9	5
39	Photoabsorption spectrum of helium trimer cationâ€"Theoretical modeling. Journal of Chemical Physics, 2013, 139, 204310.	3.0	5
40	Ligand effects on single-electron transfer of isolated iron atoms in the gaseous complexes [(OC)mFe(OH2)n]+ (m, n=0â€"2, m+n=1, 2). International Journal of Mass Spectrometry, 2012, 330-332, 95-99.	1.5	4
41	Graphene: Thiofluorographeneâ€"Hydrophilic Graphene Derivative with Semiconducting and Genosensing Properties (Adv. Mater. 14/2015). Advanced Materials, 2015, 27, 2407-2407.	21.0	4
42	Influence of ambient gas pressure and carbon adsorption on dark current emission from a cathode. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2016, 34, .	1.2	4
43	Photoabsorption spectra of small <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si33.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>He</mml:mtext></mml:mrow><mml:mrow><mml:mi>N</mml:mi></mml:mrow></mml:msubsup></mml:mrow></mml:math>		