Michael Springborg

List of Publications by Year
in descending order

67 papers	779 citations	516710 16 h-index	552781 26 g-index
70 all docs	70 docs citations	70 times ranked	806 citing authors

#	Article	IF	Citations
1	Theoretical Determination of the Most Stable Structures of Ni_mAg_n Bimetallic Nanoalloys. Journal of Physical Chemistry C, 2011, 115, 7179-7192.	3.1	64
2	Global Minimum Structures and Magic Clusters of Cu_mAg_n Nanoalloys. Journal of Physical Chemistry C, 2011, 115, 22148-22162.	3.1	64
3	Performance of Hybrid DFT Compared to MP2 Methods in Calculating Nonlinear Optical Properties of Divinylpyrene Derivative Molecules. Journal of Physical Chemistry A, 2016, 120, 8843-8852.	2.5	43
4	Efficient vector potential method for calculating electronic and nuclear response of infinite periodic systems to finite electric fields. Journal of Chemical Physics, 2007, 126, 104107.	3.0	38
5	Theoretical study of structural, electronic, and optical properties ofZnmSenclusters. Physical Review B, 2006, 73, .	3.2	35
6	Structure and energetics of nickel, copper, and gold clusters. European Physical Journal D, 2005, 34, 187-190.	1.3	34
7	Unbiased Determination of Structural and Electronic Properties of Gold Clusters with up to 58 Atoms. Journal of Physical Chemistry C, 2007, 111, 12528-12535.	3.1	34
8	The Effects of Organisation, Embedding and Surfactants on the Properties of Cadmium Chalcogenide (CdS, CdSe and CdS/CdSe) Semiconductor Nanoparticles. European Journal of Inorganic Chemistry, 2005, 2005, 3585-3596.	2.0	33
9	Theoretical Study of the Structure and Energetics of Silver Clusters. Journal of Physical Chemistry C, 2007, 111, 12577-12587.	3.1	32
10	Global structure optimization study on Au 2-20. European Physical Journal D, 2007, 43, 15-18.	1.3	32
11	Analysis of vector potential approach for calculating linear and nonlinear responses of infinite periodic systems to a finite static external electric field. Physical Review B, 2008, 77, .	3.2	32
12	Density Functional Theory Descriptors for Ionic Liquids and the Charge-Transfer Interpretation of the Haven Ratio. Journal of Physical Chemistry A, 2019, 123, 851-861.	2.5	22
13	Termination effects in electric field polarization of periodic quasi-one-dimensional systems. Physical Review B, 2010, 82, .	3.2	19
14	Solvent effects on the absorption/emission spectra of an organic chromophore: A theoretical study. Computational and Theoretical Chemistry, 2008, 866, 15-20.	1.5	17
15	How much can donor/acceptor-substitution change the responses of long pushâ€“pull systems to DC fields?. Chemical Physics Letters, 2008, 454, 105-113.	2.6	16
16	From properties to materials: An efficient and simple approach. Journal of Chemical Physics, 2017, 147, 234105.	3.0	16
17	Density Functional Theory Descriptors for Ionic Liquids and the Introduction of a Coulomb Correction. Journal of Physical Chemistry A, 2019, 123, 4188-4200.	2.5	16
18	A combined experimental and theoretical approach for structural study on a new cinnamoyl derivative of 2-acetyl-1,3-indandione and its metal(II) complexes. Structural Chemistry, 2009, 20, 101-111.	2.0	15

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19	On the dipolar electric field response of large systems. Theoretical Chemistry Accounts, 2011, 130, 687-700.	1.4	13
20	Mixed Si-Ge clusters, solar-energy harvesting, and inverse-design methods. Computational and Theoretical Chemistry, 2017, 1107, 14-22.	2.5	13
21	Structural, energetic, and electronic properties of Sin, Gen, and SinGen clusters. European Physical Journal D, 2009, 52, 39-42.	1.3	12
22	Theoretical study on the structural properties of alkali-metal heteroclusters. European Physical Journal D, 2009, 52, 35-38.	1.3	11
23	Theoretical investigation of the hydrogenation induced atomic rearrangements in palladium rich intermetallic compounds MPd3 (M = Mg, In, Tl). European Physical Journal B, 2011, 82, 1-6.	1.5	11
24	The impact of functionalization of organic semiconductors by electron donating groups on the reorganization energy. European Physical Journal D, 2019, 73, 1.	1.3	11
25	Electronic properties of Geâ€“Si nanoparticles. European Physical Journal D, 2007, 43, 213-216.	1.3	10
26	Structural and thermodynamic properties of Au2â€“20 clusters. Theoretical Chemistry Accounts, 2011, 130, 1001-1008.	1.4	10
27	Structural and energetic properties of sodium clusters. European Physical Journal D, 2007, 43, 19-22.	1.3	8
28	Electronic responses of long chains to electrostatic fields: Hartree-Fock vs. density-functional theory: A model study. Journal of Chemical Physics, 2014, 140, 054117.	3.0	8
29	Surfaces, Shapes, and Bulk Properties of Crystals. Journal of Physical Chemistry C, 2018, 122, 11926-11932.	3.1	8
30	Application of an inverse-design method to optimizing porphyrins in dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2019, 21, 5834-5844.	2.8	8
31	Surface effects on converse piezoelectricity of crystals. Physical Chemistry Chemical Physics, 2017, 19, 24724-24734.	2.8	7
32	Elemental chains. International Journal of Quantum Chemistry, 2009, 109, 837-848.	2.0	6
33	Growth patterns and structural motifs of cadmium clusters with up to 60 atoms: disordered or not?. Physical Chemistry Chemical Physics, 2016, 18, 28524-28537.	2.8	6
34	Magnetostructural phase transition assisted by temperature in Agâ€“Î±MnO₂: a density functional theory study. Physical Chemistry Chemical Physics, 2016, 18, 7442-7448.	2.8	6
35	Theoretical study of the structural and energetic properties of platinum clusters with up to 60 atoms. Structural Chemistry, 2021, 32, 469-479.	2.0	6
36	Energetic, Structural, and Vibrational Properties of 4,4â€²-Methylenediphenyl Diisocyanate with Relevance for Adhesion. Journal of Physical Chemistry A, 2016, 120, 4256-4266.	2.5	5

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37	Growth patterns, shapes, and electronic properties of mixed Si m Ge n clusters with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si58.gif" overflow="scroll"><mml:mrow><mml:mi>n</mml:mi><mml:mo>+</mml:mo><mml:mi>m</mml:mi><mml:mo>â©½</mml:mo><mml:mn Computational and Theoretical Chemistry, 2017, 1107, 30-48.	2.5	5
38	Computational study of the reactivity of cytosine derivatives. Journal of Computational Chemistry, 2017, 38, 1049-1056.	3.3	5
39	Reactivity descriptors for DNA bases and the methylation of cytosine. International Journal of Quantum Chemistry, 2018, 118, e25538.	2.0	5
40	Theoretical study of the mechanism behind the site- and enantio-selectivity of Câ€“H functionalization catalysed by chiral dirhodium catalyst. Physical Chemistry Chemical Physics, 2020, 22, 9561-9572.	2.8	5
41	Structural, Energetic, and Magnetic Properties of Ag $$_{n-m}$$ n - m Rh $$_{m}$$ m and Ag $$_{m}$$ m Rh $$_{n-m}$$ n - m Clusters with $$n le 20$$ n â‰¤ 20 and $$m=0,1$$ m = 0 , 1. Journal of Cluster Science, 2016, 27, 913-933.	3.3	4
42	Electronic orbital response of regular extended and infinite periodic systems to magnetic fields. I. Theoretical foundations for static case. Journal of Chemical Physics, 2017, 147, 104101.	3.0	4
43	Global Optimization of Li and Na Clusters: Application of a Modified Embedded Atom Method. Journal of Cluster Science, 2020, 31, 769-790.	3.3	4
44	Deposition of Ni 13 and Cu 13 clusters on Ni(111) and Cu(111) surfaces. European Physical Journal D, 2007, 45, 425-431.	1.3	3
45	Shape dependence of optical properties of sodium clusters. Applied Physics B: Lasers and Optics, 2013, 112, 177-184.	2.2	3
46	On the response of large systems to electrostatic fields. , 2012, , .		2
47	Temperature Dependence of Stability of Copper Clusters. Zeitschrift Fur Physikalische Chemie, 2016, 230, 1037-1055.	2.8	2
48	Ultranarrow heterojunctions of armchair-graphene nanoribbons as resonant-tunnelling devices. Physical Chemistry Chemical Physics, 2019, 21, 24867-24875.	2.8	2
49	Theoretical Treatment for Properties of Surfaces and Their Interplay with Bulk Properties of Crystals. Advanced Theory and Simulations, 2019, 2, 1800117.	2.8	2
50	Optimizing small conjugated molecules for solar-cell applications using an inverse-design method. Journal of Molecular Graphics and Modelling, 2020, 100, 107654.	2.4	2
51	Course on the Use of DFT Calculations to Improve Understanding of Phase Diagrams in Solid-State Chemistry. Journal of Chemical Education, 2021, 98, 3207-3217.	2.3	2
52	Structure and stability of propellane-like E 2 E 2 â€². Journal of Molecular Modeling, 2018, 24, 190.	1.8	1
53	$$hbox {Ag}_{m} hbox {Rh}_n$$ clusters with $$m+nle 55$$. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1
54	Silver hollandite (AgxMn8O16 , xâ‰2): A highly anisotropic half-metal for spintronics. Physical Review Materials, 2021, 5, .	2.4	1

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55	Role of the Backbone when Optimizing Functional Groupsâ”€A Theoretical Study Based on an Improved Inverse-Design Approach. Journal of Physical Chemistry A, 2022, 126, 1289-1299.	2.5	1
56	DFT evaluation of structural, electronic and variation properties for complex carbohydrates with biological interest. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5981-5989.	3.5	1
57	Infinite and finite solids. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 2077-2077.	1.2	0
58	Some continuous geometry transitions and the consequences for a transition-metal atom. International Journal of Quantum Chemistry, 2007, 107, 1073-1084.	2.0	0
59	Structural Responses of Infinite Periodic Systems to Electrostatic Fields. , 2009, , .		0
60	Effect of Substitution at the Ends of Long Chains on their Responses to Electrostatic Fields. , 2009, , .		0
61	L'Oeuvre of Bernie Kirtman. , 2012, , .		0
62	On the dependence of bulk properties on surfaces. , 2012, , .		0
63	Determining the size dependence of structural properties of clusters. , 2012, , .		0
64	Clusters: From trimers to nanoparticles. AIP Conference Proceedings, 2015, , .	0.4	0
65	Calculation of electron binding energies of $$hbox {Na}_{55}^-$$ Na 55 - clusters. Applied Physics B: Lasers and Optics, 2016, 122, 1.	2.2	0
66	Mechanistic Details and Conformational Behavior of Selective Peptide Linkage Facilitated by Au_n Clusters. ChemistrySelect, 2020, 5, 8352-8362.	1.5	0
67	Kinetics and Thermodynamics of CO Oxidation by (TiO2)6. Molecules, 2021, 26, 6415.	3.8	0