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	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
2	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
3	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
4	$$hbox {Ag}_{m} hbox {Rh}_n$$ clusters with $$m+nle 55$$. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1
5	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
6	Silver hollandite (AgxMn8O16 , xâ‰2): A highly anisotropic half-metal for spintronics. Physical Review Materials, 2021, 5, .	2.4	1
7	Kinetics and Thermodynamics of CO Oxidation by (TiO2)6. Molecules, 2021, 26, 6415.	3.8	0
8	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
9	Mechanistic Details and Conformational Behavior of Selective Peptide Linkage Facilitated by Au_n Clusters. ChemistrySelect, 2020, 5, 8352-8362.	1.5	0
10	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
11	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
12	Ultranarrow heterojunctions of armchair-graphene nanoribbons as resonant-tunnelling devices. Physical Chemistry Chemical Physics, 2019, 21, 24867-24875.	2.8	2
13	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
14	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
15	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
16	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
17	Theoretical Treatment for Properties of Surfaces and Their Interplay with Bulk Properties of Crystals. Advanced Theory and Simulations, 2019, 2, 1800117.	2.8	2
18	Reactivity descriptors for DNA bases and the methylation of cytosine. International Journal of Quantum Chemistry, 2018, 118, e25538.	2.0	5

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19	Surfaces, Shapes, and Bulk Properties of Crystals. Journal of Physical Chemistry C, 2018, 122, 11926-11932.	3.1	8
20	Structure and stability of propellane-like E 2 E 2 â€². Journal of Molecular Modeling, 2018, 24, 190.	1.8	1
21	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
22	Computational study of the reactivity of cytosine derivatives. Journal of Computational Chemistry, 2017, 38, 1049-1056.	3.3	5
23	Surface effects on converse piezoelectricity of crystals. Physical Chemistry Chemical Physics, 2017, 19, 24724-24734.	2.8	7
24	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
25	Mixed Si-Ge clusters, solar-energy harvesting, and inverse-design methods. Computational and Theoretical Chemistry, 2017, 1107, 14-22.	2.5	13
26	From properties to materials: An efficient and simple approach. Journal of Chemical Physics, 2017, 147, 234105.	3.0	16
27	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
28	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
29	Calculation of electron binding energies of $$hbox {Na}_{55}^-$$ Na 55 - clusters. Applied Physics B: Lasers and Optics, 2016, 122, 1.	2.2	0
30	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
31	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
32	Temperature Dependence of Stability of Copper Clusters. Zeitschrift Fur Physikalische Chemie, 2016, 230, 1037-1055.	2.8	2
33	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
34	Clusters: From trimers to nanoparticles. AIP Conference Proceedings, 2015, , .	0.4	0
35	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
36	Shape dependence of optical properties of sodium clusters. Applied Physics B: Lasers and Optics, 2013, 112, 177-184.	2.2	3

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37	L'Oeuvre of Bernie Kirtman. , 2012, , .		0
38	On the dependence of bulk properties on surfaces. , 2012, , .		0
39	Determining the size dependence of structural properties of clusters. , 2012, , .		0
40	On the response of large systems to electrostatic fields. , 2012, , .		2
41	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
42	Global Minimum Structures and Magic Clusters of Cu_mAg_n Nanoalloys. Journal of Physical Chemistry C, 2011, 115, 22148-22162.	3.1	64
43	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
44	On the dipolar electric field response of large systems. Theoretical Chemistry Accounts, 2011, 130, 687-700.	1.4	13
45	Structural and thermodynamic properties of Au2â€“20 clusters. Theoretical Chemistry Accounts, 2011, 130, 1001-1008.	1.4	10
46	Termination effects in electric field polarization of periodic quasi-one-dimensional systems. Physical Review B, 2010, 82, .	3.2	19
47	Structural Responses of Infinite Periodic Systems to Electrostatic Fields. , 2009, , .		0
48	Effect of Substitution at the Ends of Long Chains on their Responses to Electrostatic Fields. , 2009, , .		0
49	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
50	Elemental chains. International Journal of Quantum Chemistry, 2009, 109, 837-848.	2.0	6
51	Structural, energetic, and electronic properties of Sin, Gen, and SinGen clusters. European Physical Journal D, 2009, 52, 39-42.	1.3	12
52	Theoretical study on the structural properties of alkali-metal heteroclusters. European Physical Journal D, 2009, 52, 35-38.	1.3	11
53	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
54	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

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55	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
56	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
57	Theoretical Study of the Structure and Energetics of Silver Clusters. Journal of Physical Chemistry C, 2007, 111, 12577-12587.	3.1	32
58	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
59	Some continuous geometry transitions and the consequences for a transition-metal atom. International Journal of Quantum Chemistry, 2007, 107, 1073-1084.	2.0	0
60	Electronic properties of Geâ€“Si nanoparticles. European Physical Journal D, 2007, 43, 213-216.	1.3	10
61	Global structure optimization study on Au 2-20. European Physical Journal D, 2007, 43, 15-18.	1.3	32
62	Structural and energetic properties of sodium clusters. European Physical Journal D, 2007, 43, 19-22.	1.3	8
63	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
64	Infinite and finite solids. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 2077-2077.	1.2	0
65	Theoretical study of structural, electronic, and optical properties ofZnmSenclusters. Physical Review B, 2006, 73, .	3.2	35
66	Structure and energetics of nickel, copper, and gold clusters. European Physical Journal D, 2005, 34, 187-190.	1.3	34
67	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