

Capturing a Synergistic Effect of a Conical Push and an
of $\text{Li}@B_{10}H_{14}$ Basket: Toward
Potential and Nonlinear Optical Response

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Density Functional Theory Investigation on the Second-Order Nonlinear Optical Properties of Chlorobenzyl- <i>o</i> -Carborane Derivatives. Chinese Journal of Chemistry, 2012, 30, 2349-2355.	2.6	10
2	Halide Ion Complexes of Decaborane (B ₁₀ H ₁₄) and Their Derivatives: Noncovalent Charge Transfer Effect on Second-Order Nonlinear Optical Properties. Journal of Physical Chemistry A, 2012, 116, 1417-1424.	1.1	62
3	The stability and nonlinear optical properties: Encapsulation of an excess electron compound LiCN ⁻ Li within boron nitride nanotubes. Journal of Materials Chemistry, 2012, 22, 2196-2202.	6.7	111
4	THEORETICAL INVESTIGATION ON SECOND-ORDER NONLINEAR OPTICAL PROPERTIES AND REDOX-SWITCHING OF PHENYL NITRONYL-NITROXIDE RADICAL DERIVATIVES. Journal of Theoretical and Computational Chemistry, 2012, 11, 1075-1088.	1.8	5
5	The Excess Electron in a Boron Nitride Nanotube: Pyramidal NBO Charge Distribution and Remarkable First Hyperpolarizability. Chemistry - A European Journal, 2012, 18, 11350-11355.	1.7	87
6	Quantum chemical design of nonlinear optical materials by sp ² -hybridized carbon nanomaterials: issues and opportunities. Journal of Materials Chemistry C, 2013, 1, 5439.	2.7	155
7	The encapsulated lithium effect of Li@C ₆₀ Cl ₈ remarkably enhances the static first hyperpolarizability. RSC Advances, 2013, 3, 13348.	1.7	19
8	Structures and redox-switchable second-order nonlinear optics properties of N-legged piano stool shaped 12-vertex rhenacarborane half-sandwich complexes. Journal of Organometallic Chemistry, 2013, 728, 6-15.	0.8	13
9	A new type of organic-inorganic hybrid NLO-phore with large off-diagonal first hyperpolarizability tensors: a two-dimensional approach. Dalton Transactions, 2013, 42, 15053.	1.6	111
10	Temperature dependence of nonlinear optical properties in Li doped nano-carbon bowl material. Applied Physics Letters, 2013, 102, 153307.	1.5	11
11	Li doped effect of through novel noncovalent charge transfer on nonlinear optical properties. Dyes and Pigments, 2014, 106, 7-13.	2.0	31
12	Helical Carbon Segment in Carbon-Boron-Nitride Heteronanotubes: Structure and Nonlinear Optical Properties. ChemPlusChem, 2014, 79, 732-736.	1.3	16
13	Multilithiation Effect on the First Hyperpolarizability of Carbon-Boron-Nitride Heteronanotubes: Activating Segment versus Connecting Pattern. Journal of Physical Chemistry C, 2014, 118, 14185-14191.	1.5	33
14	Suitable helical cavity, suitable alkali metal, larger first hyperpolarizability. Chemical Physics Letters, 2014, 600, 123-127.	1.2	4
15	Second-order nonlinear optical properties of dithienophenazine and TTF derivatives: A butterfly effect of dimalonitrile substitutions. Journal of Molecular Graphics and Modelling, 2015, 59, 14-20.	1.3	47
16	Theoretical insights and design of intriguing nonlinear optical species involving the excess electron. International Journal of Quantum Chemistry, 2015, 115, 671-679.	1.0	41
17	Experimental and density functional theory (DFT): A dual approach to study the various important properties of monohydrated l-proline cadmium chloride for nonlinear optical applications. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 143, 128-135.	2.0	41
18	Role of Excess Electrons in Nonlinear Optical Response. Journal of Physical Chemistry Letters, 2015, 6, 612-619.	2.1	181

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19	One lithium atom binding with P-nitroaniline: lithium salts or lithium electrides?. Journal of Molecular Modeling, 2015, 21, 23.	0.8	11
20	Nonlinear optical properties of rhenium(I) complexes: Influence of the extended π -conjugated connectors and proton abstraction. Journal of Molecular Graphics and Modelling, 2015, 61, 196-203.	1.3	7
21	Combined experimental and computational insights into the key features of α -alanine α -alaninium picrate monohydrate: growth, structural, electronic and nonlinear optical properties. RSC Advances, 2015, 5, 53988-54002.	1.7	29
22	The influence of alkali metals (Li, Na and K) interaction with Be ₁₂ O ₁₂ and Mg ₁₂ O ₁₂ nanoclusters on their structural, electronic and nonlinear optical properties: A theoretical study. Synthetic Metals, 2015, 204, 17-24.	2.1	58
23	Second-Order Nonlinear Optical Response of Electron Donor-Acceptor Hybrids Formed between Corannulene and Metallofullerenes. Journal of Physical Chemistry C, 2015, 119, 24965-24975.	1.5	60
24	A dual approach to study the electro-optical properties of a noncentrosymmetric L-asparagine monohydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 432-441.	2.0	37
25	Tuning the push-pull configuration for efficient second-order nonlinear optical properties in some chalcone derivatives. Journal of Molecular Graphics and Modelling, 2016, 68, 95-105.	1.3	77
26	A theoretical study of the spectroscopic properties of benzene and of a series of $C_{2n}H_{2n}$ species ($x\hat{A}=1\hat{A}^{12}$, $y\hat{A}=3\hat{A}^{14}$, $z\hat{A}=0\hat{A}^{2}$): From BH ₃ to B ₁₂ . International Journal of Hydrogen Energy, 2016, 41, 13954-13959.	3.8	31
27	Connecting effect on the first hyperpolarizability of armchair carbon-boron nitride heteronanotubes: pattern versus proportion. Physical Chemistry Chemical Physics, 2016, 18, 13954-13959.	1.3	17
28	M@B ₄₀ (M = Li, Na, K) serving as a potential promising novel NLO nanomaterial. Chemical Physics Letters, 2016, 654, 76-80.	1.2	71
29	The interaction between Boron-carbon-nitride heteronanotubes and lithium atoms: Role of composition proportion. Chemical Physics Letters, 2016, 658, 230-233.	1.2	6
30	Theoretical study of the non linear optical properties of alkali metal (Li, Na, K) doped aluminum nitride nanocages. RSC Advances, 2016, 6, 94228-94235.	1.7	62
31	Are phosphide nano-cages better than nitride nano-cages? A kinetic, thermodynamic and non-linear optical properties study of alkali metal encapsulated X ₁₂ Y ₁₂ nano-cages. Journal of Materials Chemistry C, 2016, 4, 10919-10934.	2.7	122
32	12-vertex ruthenacarborane half-sandwich complexes: Redox properties and second-order nonlinear optical responses. Journal of Organometallic Chemistry, 2016, 801, 54-59.	0.8	4
33	A quantum chemical study on the remarkable nonlinear optical and electronic characteristics of boron nitride nanoclusters by complexation via lithium atom. Journal of Molecular Liquids, 2016, 221, 443-451.	2.3	32
34	The impact of position and number of methoxy group(s) to tune the nonlinear optical properties of chalcone derivatives: a dual substitution strategy. Journal of Molecular Modeling, 2016, 22, 73.	0.8	39
35	Theoretical assessment of the electro-optical features of the group III nitrides (B ₁₂ N ₁₂ , Al ₁₂ N ₁₂ and Tl ₁₂ N ₁₂) with alkali metals (Li, Na and K). Applied Surface Science, 2016, 363, 197-208.	3.1	83
36	The influence of Sc doping on structural, electronic and optical properties of Be ₁₂ O ₁₂ , Mg ₁₂ O ₁₂ and Ca ₁₂ O ₁₂ nanocages: a DFT study. Journal of Molecular Modeling, 2017, 23, 82.	0.8	21

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37	A computational study on the electro-optical characteristics of C _{2n} (BN) 12-n (n = 1–11) hetero-nanoclusters: Toward the remarkable features by the encapsulation via alkali metals. <i>Journal of Molecular Liquids</i> , 2017, 233, 236-242.	2.3	4
38	Li _n @B ₃₆ (n = 1, 2) Nanosheet with Remarkable Electro-Optical Properties: A DFT Study. <i>Journal of Electronic Materials</i> , 2017, 46, 4420-4425.	1.0	14
39	Theoretical investigation on second-order nonlinear optical properties of ruthenium alkynyl-dihydroazulene/vinylheptafulvene complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 363-371.	1.3	3
40	The important role of superalkalis on the static first hyperpolarizabilities of new electrides: Theoretical investigation on superalkali-doped hexamethylenetetramine (HMT). <i>Synthetic Metals</i> , 2017, 232, 39-45.	2.1	25
41	Effect of Doped Transition Metal Atoms on Structure and Nonlinear Optical Properties of Decaborane. <i>Journal of Electronic Materials</i> , 2017, 46, 6347-6356.	1.0	7
42	Structural, electrical and optical properties of Li _n @C ₂₀ (n = 1–6) nanoclusters. <i>Comptes Rendus Chimie</i> , 2018, 21, 541-546.	0.2	16
43	Transition metal doping: a new and effective approach for remarkably high nonlinear optical response in aluminum nitride nanocages. <i>New Journal of Chemistry</i> , 2018, 42, 6976-6989.	1.4	61
44	Copper-doped Al ₁₂ N ₁₂ nano-cages: potential candidates for nonlinear optical materials. <i>Applied Physics A: Materials Science and Processing</i> , 2018, 124, 1.	1.1	38
45	The Effect of Superalkali M ₃ O (M = Li, Na and K) on Structure, Electrical and Nonlinear Optical Properties of C ₂₀ Fullerene Nanocluster. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2018, 28, 110-120.	1.9	12
46	A Complex Containing Four Magnesium Atoms and Two Mg–Mg Bonds Behaving as an Electride. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4105-4111.	1.0	15
47	Calculation of Vibrational Parameters of an Electride-Like Molecule Li ₄ C ₄ H ₂ N ₂ and the Pyridazine Molecule C ₄ H ₄ N ₂ . <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2019, 127, 218-224.	0.2	1
48	Effect of B, Al and Ga atoms on structures, electrical and optical properties of BeO nanotube. <i>ChemistrySelect</i> , 2019, 4, 6739-6743.	0.7	1
49	A theoretical study of alkaline-earthides Li(NH ₃) ₄ M (M = Be, Mg, Ca) with large first hyperpolarizability. <i>Journal of Molecular Modeling</i> , 2019, 25, 150.	0.8	24
50	Investigations of electronic and nonlinear optical properties of single alkali metal adsorbed graphene, graphyne and graphdiyne systems by first-principles calculations. <i>Journal of Materials Chemistry C</i> , 2019, 7, 1630-1640.	2.7	101
51	A dual approach to study the key features of nickel (II) and copper (II) coordination complexes: Synthesis, crystal structure, optical and nonlinear properties. <i>Inorganica Chimica Acta</i> , 2019, 484, 148-159.	1.2	39
52	Alkaline earth metal decorated phosphide nanoclusters for potential applications as high performance NLO materials; A first principle study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 118, 113906.	1.3	38
53	Electronic and nonlinear optical features of first row transition metals-decorated all-boron B ₄₀ fullerene: A promising route to remarkable electro-optical response. <i>Inorganic Chemistry Communication</i> , 2020, 112, 107692.	1.8	15
54	Assessing the structure and first hyperpolarizability of Li@B ₁₀ H ₁₄ in solution: a sequential QM/MM study using the ASE-CFEG method. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17314-17324.	1.3	8

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55	Electride Characteristics of Some Binuclear Sandwich Complexes of Alkaline Earth Metals, $M_{2}(\bar{L})_{5}L_{2}$ ($M = Be, Mg; L =$) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 742 Td ($C_{5}H_{17}$)	1.1	17
56	Enhanced electronic and nonlinear optical responses of $C_{24}N_{24}$ cavernous nitride fullerene by decoration with first row transition metals; A computational investigation. Applied Organometallic Chemistry, 2020, 34, e5694.	1.7	23
57	Encapsulation of Mg_{2} inside a C_{60} cage forms an electride. Journal of Computational Chemistry, 2020, 41, 1645-1653.	1.5	20
58	Enhanced linear and nonlinear optical response of superhalogen (Al ₇) doped graphitic carbon nitride (g-C ₃ N ₄). Optik, 2021, 226, 165923.	1.4	46
59	First row transition metals decorated boron phosphide nanoclusters as nonlinear optical materials with high thermodynamic stability and enhanced electronic properties; A detailed quantum chemical study. Optics and Laser Technology, 2021, 134, 106570.	2.2	34
60	Influence of alkali metal atoms on structure, electronic and non-linear optical properties of calix[4]arene. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 127, 114539.	1.3	3
61	Comparison Between Electride Characteristics of Li ₃ @B ₄₀ and Li ₃ @C ₆₀ . Frontiers in Chemistry, 2021, 9, 638581.	1.8	11
62	Nonlinear optical response of teetotum boron clusters. Computational and Theoretical Chemistry, 2021, 1198, 113178.	1.1	7
63	Electride characteristics of $M_{2}(\bar{E})_{5}E_{2}$ ($M = Be, Mg; E = Sb^{5-}$). Structural Chemistry, 2021, 32, 2107-2114.	1.0	5
64	Atomic Clusters: Structure, Reactivity, Bonding, and Dynamics. Frontiers in Chemistry, 2021, 9, 730548.	1.8	14
65	Design a novel type of excess electron compounds with large nonlinear optical responses using group 12 elements (Zn, Cd and Hg). Journal of Molecular Graphics and Modelling, 2021, 109, 108003.	1.3	4
66	From an electride-like super alkali earth atom to a superalkalide or superalkali electride: $M(HF)_{3}M$ ($M = Na$ or Li) as field-induced excellent inorganic NLO molecular switches. Journal of Materials Chemistry C, 2021, 9, 14885-14896.	2.7	13
67	Insighting the functionally modified C ₆₀ fullerenes as an efficient nonlinear optical materials: A quantum chemical study. Materials Science in Semiconductor Processing, 2022, 141, 106421.	1.9	17
68	Quantum design of transition metals decorated on boron phosphide inorganic nanocluster for Favipiravir adsorption: a possible treatment for COVID-19. New Journal of Chemistry, 2022, 46, 1720-1730.	1.4	13
69	Stabilisation of Li(0)-Li(0) bond by normal and mesoionic carbenes and electride characteristics of the complexes. Molecular Physics, 2022, 120, .	0.8	4
70	Molecular Electrides: An In Silico Perspective. ChemPhysChem, 2022, 23, .	1.0	4
71	DFT study of super-halogen (Al ₇) doped carbon nitride (C ₂ N) and its nonlinear optical properties. Journal of Molecular Structure, 2022, 1270, 133910.	1.8	4
72	Molecular electrides: An overview of their structure, bonding, and reactivity. , 2023, , 275-295.		0

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73	Structure, Stability, Bonding and Aromaticity in All-metal and Nonmetal Clusters. , 2024, , 471-481.		0
74	Nonlinear optical properties of superalkali@teetotum boron clusters with potential applications on the electro-optic modulator. Computational and Theoretical Chemistry, 2023, 1223, 114078.	1.1	1
75	Conformational Dependence of the First Hyperpolarizability of the Li@B10H14 in Solution. Liquids, 2023, 3, 159-167.	0.8	0