

Junais Habeeb Mokkaath

List of Publications by Year in descending order

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Version: 2024-02-01

82
papers

504
citations

759055

12
h-index

839398

18
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82
all docs

82
docs citations

82
times ranked

475
citing authors

#	ARTICLE	IF	CITATIONS
1	First-principles study of structural, magnetic, and electronic properties of small Fe-Rh alloy clusters. <i>Physical Review B</i> , 2012, 85, .	1.1	42
2	Computational Study of Magic-Size CdSe Clusters with Complementary Passivation by Carboxylic and Amine Ligands. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10015-10019.	1.5	32
3	One-dimensional aluminum nanoparticle chains: the influence of interparticle spacing and chain length on plasmon coupling behavior. <i>Journal of Materials Chemistry C</i> , 2017, 5, 4379-4383.	2.7	27
4	Interplay between Chemical and Magnetic Order in FeRh Clusters. <i>Journal of Physical Chemistry C</i> , 2012, 116, 17228-17238.	1.5	26
5	Shapes matter: examining the optical response evolution in stretched aluminium nanoparticles via time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 51-55.	1.3	24
6	Tuning the chemical activity through PtAu nanoalloying: a first principles study. <i>Journal of Materials Chemistry A</i> , 2013, 1, 9885.	5.2	19
7	Structural and Optical Properties of Si-Doped Ag Clusters. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4885-4889.	1.5	15
8	Tuning the optical response in carbon doped boron nitride nanodots. <i>Journal of Materials Chemistry C</i> , 2014, 2, 8322-8327.	2.7	14
9	An asymmetric aluminum active quantum plasmonic device. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1416-1421.	1.3	14
10	Photoabsorption Spectra of (Mo/W) ₁₂ Si ₆₀ Clusters from Time-Dependent DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23938-23941.	1.5	13
11	Magnetism, structure and chemical order in small CoPd clusters: A first-principles study. <i>Journal of Magnetism and Magnetic Materials</i> , 2014, 349, 109-115.	1.0	13
12	Ultraviolet plasmon resonance in transition-metal doped aluminum nanoparticle arrays. <i>Journal of Materials Chemistry C</i> , 2018, 6, 2225-2228.	2.7	13
13	Linear acene molecules in plasmonic cavities: mapping evolution of optical absorption spectra and electric field intensity enhancements. <i>New Journal of Chemistry</i> , 2019, 43, 10774-10783.	1.4	13
14	Dopant-induced localized light absorption in CsPbX ₃ (X = Cl, Br, I) perovskite quantum dots. <i>New Journal of Chemistry</i> , 2019, 43, 18268-18276.	1.4	13
15	Localized surface plasmon resonances and electric field confinement in titanium carbide (Ti ₃ C ₂) MXene nanoclusters. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25807-25816.	1.3	13
16	Localized surface plasmon resonances in a hybrid structure consisting of a mono-layered Al sheet and Ti ₃ C ₂ F MXene. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12389-12396.	1.3	13
17	Exotic High Activity Surface Patterns in PtAu Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2013, 117, 9275-9280.	1.5	10
18	Tunable optical absorption in silicene molecules. <i>Journal of Materials Chemistry C</i> , 2016, 4, 7387-7390.	2.7	10

#	ARTICLE	IF	CITATIONS
19	Nanometer size 3d ⁴ and 3d ⁵ substitutional clusters: Promising candidates for magnetic storage applications. Journal of Magnetism and Magnetic Materials, 2013, 334, 31-35.	1.0	9
20	Strain induced plasmon tuning in planar square-shaped aluminum nanoparticles array. Chemical Physics Letters, 2018, 702, 102-105.	1.2	9
21	Water-calcite (104) surface interactions using first-principles simulations. Journal of Physics and Chemistry of Solids, 2022, 161, 110394.	1.9	9
22	Catalytically favorable surface patterns in Pt ⁴ Au nanoclusters. RSC Advances, 2013, 3, 15350.	1.7	8
23	Competing plasmonic and charge-transfer excitations in pyridine adsorbed silver and aluminum nanoparticles. Physical Chemistry Chemical Physics, 2018, 20, 15884-15889.	1.3	7
24	Optical properties of Al nanostructures from time dependent density functional theory. Journal of Chemical Physics, 2016, 144, 134305.	1.2	6
25	Nanoparticle heterodimers: The role of size and interparticle gap distance on the optical response. Chemical Physics Letters, 2018, 699, 28-31.	1.2	6
26	Band edge optical properties of defected MoS ₂ nanotubes. Chemical Physics Letters, 2018, 706, 641-646.	1.2	6
27	Photo-induced electron transfer between a metal nanoparticle and a collection of molecular emitters. Chemical Physics Letters, 2020, 758, 137905.	1.2	6
28	Observation of robust infrared plasmons in twisted titanium carbide (Ti ₃ C ₂) MXene. Journal of Physics and Chemistry of Solids, 2022, 164, 110612.	1.9	6
29	Magnetic Phase Transition in 2 nm Ni _x Cu _{1-x} (0 ≤ x ≤ 1) Clusters. Journal of Physical Chemistry C, 2014, 118, 8169-8173.	1.5	5
30	Chemical ordering patterns and magnetism of NiAl nanoclusters. Materials Research Express, 2017, 4, 015010.	0.8	5
31	Strong Collectivity of Optical Transitions in Lead Halide Perovskite Quantum Dots. Plasmonics, 2020, 15, 581-590.	1.8	5
32	Size and chemical order dependence of magnetic-ordering temperature and spin structure in Fe@Ni and Ni@Fe core-shell nanoparticles. Physical Chemistry Chemical Physics, 2020, 22, 6275-6281.	1.3	5
33	Temperature-dependent electronic structure of bixbyite $\hat{\pm}$ -Mn ₂ O ₃ and the importance of a subtle structural change on oxygen electrocatalysis. Science and Technology of Advanced Materials, 2021, 22, 141-149.	2.8	5
34	Gd doped Au nanoclusters: Molecular magnets with novel properties. Chemical Physics Letters, 2014, 592, 217-221.	1.2	4
35	Absorption Spectra of CuGaSe ₂ and CuInSe ₂ Semiconducting Nanoclusters. Journal of Physical Chemistry C, 2015, 119, 22732-22736.	1.5	4
36	Plasmon coupling behavior in aluminium nanoparticle arrangements. Journal of Materials Chemistry C, 2016, 4, 10616-10619.	2.7	4

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37	Exotic chemical arrangements and magnetic moment evolution of Ni		

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55	Skyrmion formation and dynamics in magnetic bilayers via atomistic spin dynamics simulations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 130, 114720.	1.3	2
56	Effect of the interplay between layering sequence permutations and thickness on the magnetic features of Fe/Ni/Gd hetero-films. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12082-12091.	1.3	2
57	Mapping nanoscale electric field hotspots of a plasmon-molecule system: A theoretical study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 137, 115055.	1.3	2
58	Optical properties of core-shell and multi-shell nanorods. <i>Chemical Physics Letters</i> , 2018, 699, 188-193.	1.2	1
59	Optical properties of magnesium nanorods using time dependent density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28903-28909.	1.3	1
60	Optical properties of bimetallic compositional heterodimers. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19017-19022.	1.3	1
61	Plasmons of hollow nanobar oligomers. <i>New Journal of Chemistry</i> , 2019, 43, 12351-12357.	1.4	1
62	Probing role of shell thickness in the optical response of core-shell nanorods. <i>Chemical Physics Letters</i> , 2019, 717, 175-181.	1.2	1
63	Optical resonance coupling in compositionally different nanocube-nanosphere heterodimers. <i>New Journal of Chemistry</i> , 2019, 43, 6959-6964.	1.4	1
64	Optical properties of aluminum intercalated magnesium nanoparticle square array: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6750-6755.	1.3	1
65	A quantum mechanical study of optical excitations in nanodisk plasmonic oligomers. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26540-26548.	1.3	1
66	Electric Near-field Modulations of Charged Deoxyribonucleic Acid Nucleobases. <i>Plasmonics</i> , 2020, 15, 1411-1420.	1.8	1
67	Nanoscale field enhancement of a close-packed nanoparticle cluster. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 129, 114670.	1.3	1
68	Optical features of ligated semiconducting quantum dots subjected to an electric field. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26763.	1.0	1
69	Shapes matter: examining the optical response evolution in stretched aluminium nanoparticles via time-dependent density functional theory. , 0, .		1
70	One-dimensional aluminum nanoparticle chains: the influence of interparticle spacing and chain length on plasmon coupling behavior. , 0, .		1
71	Magnetic skyrmions in monoatomic-thin Gadolinium square-shaped nanoislands. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, , 115015.	1.3	1
72	Probing the self-diffusion process in Aluminium. <i>Journal of Molecular Modeling</i> , 2022, 28, 21.	0.8	1

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73	Free Energy Surfaces and Barriers for Vacancy Diffusion on Al(100), Al(110), Al(111) Reconstructed Surfaces. <i>Nanomaterials</i> , 2022, 12, 76.	1.9	1
74	Impact of Adsorption of Straight Chain Alcohol Molecules on the Optical Properties of Calcite (10.4) Surface. <i>Nanomaterials</i> , 2022, 12, 1460.	1.9	1
75	Optical response tuning in nanorod-on-semicontinuous film systems: A computational study. <i>Chemical Physics Letters</i> , 2018, 692, 88-93.	1.2	0
76	Morphology dependent optical response tuning in planar square-shaped array of sodium nanoparticles. <i>Journal of Molecular Modeling</i> , 2018, 24, 293.	0.8	0
77	Optical Response Tuning of Compositional Heterodimers: a TDDFT Study. <i>Plasmonics</i> , 2019, 14, 539-545.	1.8	0
78	Optical excitations of boron and phosphorous doped silicon nanoparticles: A computational study. <i>Chemical Physics Letters</i> , 2019, 717, 107-111.	1.2	0
79	Charge-transfer excitons of metal intercalated pentacene dimers. <i>Chemical Physics Letters</i> , 2019, 729, 1-5.	1.2	0
80	Plasmons of magnesium nanodisks and their interactions with a dipole-carrying molecule. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 108, 296-299.	1.3	0
81	Plasmon-Molecule Coupling with Directional Absorption Features: A First-Principles Study. <i>Plasmonics</i> , 2021, 16, 1287-1296.	1.8	0
82	Electric Field Distribution of an Optical Nanocavity Embedded with a Single Molecule. <i>Plasmonics</i> , 2021, 16, 1515-1524.	1.8	0