

# Junais Habeeb Mokkath

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

78  
papers

318  
citations

9  
h-index

15  
g-index

82  
ext. papers

418  
ext. citations

3.5  
avg, IF

4.67  
L-index

#	Paper	IF	Citations
78	Observation of robust infrared plasmons in twisted titanium carbide (Ti <sub>3</sub> C <sub>2</sub> ) MXene. <i>Journal of Physics and Chemistry of Solids</i> , <b>2022</b> , 164, 110612	3.9	1
77	Water-calcite (104) surface interactions using first-principles simulations. <i>Journal of Physics and Chemistry of Solids</i> , <b>2022</b> , 161, 110394	3.9	0
76	Mapping nanoscale electric field hotspots of a plasmon-molecule system: A theoretical study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 137, 115055	3	0
75	Localized surface plasmon resonances and electric field confinement in titanium carbide (TiC) MXene nanoclusters. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 25807-25816	3.6	2
74	Magnetic skyrmions in monoatomic-thin Gadolinium square-shaped nanoislands. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 115015	3	0
73	Plasmonic properties of nanohybrids made of metallic nanoring and benzene molecules. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26646	2.1	0
72	Temperature-dependent electronic structure of bixbyite MnO and the importance of a subtle structural change on oxygen electrocatalysis. <i>Science and Technology of Advanced Materials</i> , <b>2021</b> , 22, 141-149	7.1	0
71	Nanoscale field enhancement of a close-packed nanoparticle cluster. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 129, 114670	3	0
70	Skyrmion formation and dynamics in magnetic bilayers via atomistic spin dynamics simulations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 130, 114720	3	0
69	Optical features of ligated semiconducting quantum dots subjected to an electric field. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26763	2.1	0
68	Subfemtosecond charge dynamics in vertically stacked bilayer silicene. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26521	2.1	1
67	Delocalized exciton formation in C <sub>60</sub> linear molecular aggregates. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 21901-21912	3.6	0
66	Plasmon-Molecule Coupling with Directional Absorption Features: A First-Principles Study. <i>Plasmonics</i> , <b>2021</b> , 16, 1287-1296	2.4	0
65	Electric Field Distribution of an Optical Nanocavity Embedded with a Single Molecule. <i>Plasmonics</i> , <b>2021</b> , 16, 1515-1524	2.4	0
64	Probing the self-diffusion process in Aluminium.. <i>Journal of Molecular Modeling</i> , <b>2021</b> , 28, 21	2	0
63	Size and chemical order dependence of magnetic-ordering temperature and spin structure in Fe@Ni and Ni@Fe core-shell nanoparticles. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 6275-6281	3.6	0
62	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> , <b>2020</b> , 22, 12082-12091	3.6	0

61	Strong Collectivity of Optical Transitions in Lead Halide Perovskite Quantum Dots. <i>Plasmonics</i> , <b>2020</b> , 15, 581-590	2.4	2
60	An asymmetric aluminum active quantum plasmonic device. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 1416-1421	3.6	3
59	Photo-induced electron transfer between a metal nanoparticle and a collection of molecular emitters. <i>Chemical Physics Letters</i> , <b>2020</b> , 758, 137905	2.5	2
58	IV characteristics of an atomically thin graphene-boron nitride heterostructure. <i>Chemical Physics Letters</i> , <b>2020</b> , 761, 138115	2.5	2
57	Localized surface plasmon resonances of a metal nanoring. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 23878-23885	3.6	2
56	Electric Near-field Modulations of Charged Deoxyribonucleic Acid Nucleobases. <i>Plasmonics</i> , <b>2020</b> , 15, 1411-1420	2.4	0
55	Optical excitations of boron and phosphorous doped silicon nanoparticles: A computational study. <i>Chemical Physics Letters</i> , <b>2019</b> , 717, 107-111	2.5	
54	Probing role of shell thickness in the optical response of core-shell nanorods. <i>Chemical Physics Letters</i> , <b>2019</b> , 717, 175-181	2.5	1
53	Linear acene molecules in plasmonic cavities: mapping evolution of optical absorption spectra and electric field intensity enhancements. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 10774-10783	3.6	7
52	Charge-transfer excitons of metal intercalated pentacene dimers. <i>Chemical Physics Letters</i> , <b>2019</b> , 729, 1-5	2.5	
51	Electric field hotspots of all-inorganic off-stoichiometric APbX <sub>3</sub> (A = Cs, Rb and X = Cl, Br, I) perovskite quantum dots. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2019</b> , 113, 65-71	3	1
50	Optical resonance coupling in compositionally different nanocube-nanosphere heterodimers. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 6959-6964	3.6	1
49	Probing the role of capping ligands, ligand loss and solvent effects on the optoelectronic properties of CdS quantum dots. <i>Journal of Physics and Chemistry of Solids</i> , <b>2019</b> , 131, 10-14	3.9	3
48	Optical properties of aluminum intercalated magnesium nanoparticle square array: a computational study. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 6750-6755	3.6	1
47	Optical properties of nanodisk heterodimers using quantum chemical calculations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2019</b> , 111, 226-232	3	0
46	Optical Response Tuning of Compositional Heterodimers: a TDDFT Study. <i>Plasmonics</i> , <b>2019</b> , 14, 539-545	2.4	
45	Probing Subnanometric-Scale Hotspots in Metallic Interfaces. <i>Plasmonics</i> , <b>2019</b> , 14, 2031-2043	2.4	0
44	Electric field amplification of plasmon-molecule hybrids revealed by first-principles time dependent density functional theory calculations. <i>International Journal of Quantum Chemistry</i> , <b>2019</b> , 119, e26021	2.1	2

43	Plasmons of hollow nanobar oligomers. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 12351-12357	3.6	1
42	A quantum mechanical study of optical excitations in nanodisk plasmonic oligomers. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 26540-26548	3.6	0
41	Dopant-induced localized light absorption in CsPbX <sub>3</sub> (X = Cl, Br, I) perovskite quantum dots. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 18268-18276	3.6	9
40	Plasmons of magnesium nanodisks and their interactions with a dipole-carrying molecule. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2019</b> , 108, 296-299	3	
39	Optical properties of pyridine adsorbed polycyclic aromatic hydrocarbons using quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 21, 448-454	3.6	2
38	Ultraviolet plasmon resonance in transition-metal doped aluminum nanoparticle arrays. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 2225-2228	7.1	9
37	Optical response tuning in nanorod-on-semicontinuous film systems: A computational study. <i>Chemical Physics Letters</i> , <b>2018</b> , 692, 88-93	2.5	
36	Optical response tuning in graphene nanoflakes: A computational study. <i>Chemical Physics Letters</i> , <b>2018</b> , 692, 102-105	2.5	2
35	Optical properties of core-shell and multi-shell nanorods. <i>Chemical Physics Letters</i> , <b>2018</b> , 699, 188-193	2.5	1
34	Nanoparticle heterodimers: The role of size and interparticle gap distance on the optical response. <i>Chemical Physics Letters</i> , <b>2018</b> , 699, 28-31	2.5	5
33	A quantum mechanical study of the optical response evolution in nanorod dimers. <i>Chemical Physics Letters</i> , <b>2018</b> , 696, 36-41	2.5	2
32	Exotic chemical arrangements and magnetic moment evolution of Ni <sub>x</sub> Pt <sub>1-x</sub> (0 ≤ x ≤ 1) nanoparticles. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2018</b> , 456, 269-273	2.8	3
31	Band Edge Optical Excitation of Pyridine-Adsorbed CuAg Nanoparticles. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 6467-6472	2.8	1
30	Band edge optical properties of defected MoS <sub>2</sub> nanotubes. <i>Chemical Physics Letters</i> , <b>2018</b> , 706, 641-646	2.5	4
29	Aluminum nanorods subject to bending and twisting distortions: Optical response modulations using quantum mechanical simulations. <i>Journal of Physics and Chemistry of Solids</i> , <b>2018</b> , 123, 32-35	3.9	0
28	Optical properties of magnesium nanorods using time dependent density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 28903-28909	3.6	1
27	Morphology dependent optical response tuning in planar square-shaped array of sodium nanoparticles. <i>Journal of Molecular Modeling</i> , <b>2018</b> , 24, 293	2	
26	Strain induced plasmon tuning in planar square-shaped aluminum nanoparticles array. <i>Chemical Physics Letters</i> , <b>2018</b> , 702, 102-105	2.5	5

25	Competing plasmonic and charge-transfer excitations in pyridine adsorbed silver and aluminum nanoparticles. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 15884-15889	3.6	2
24	Optical properties of bimetallic compositional heterodimers. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 19017-19022	3.6	1
23	One-dimensional aluminum nanoparticle chains: the influence of interparticle spacing and chain length on plasmon coupling behavior. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 4379-4383	7.1	23
22	Chemical ordering patterns and magnetism of NiAl nanoclusters. <i>Materials Research Express</i> , <b>2017</b> , 4, 015010	1.7	2
21	Evolution of the Magnetic and Optical Properties in Co@Au Core-Shell and (CoRh)@Au Core-Shell Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 24798-24803	3.8	3
20	Shapes matter: examining the optical response evolution in stretched aluminium nanoparticles via time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 20, 51-55	3.6	21
19	Tunable optical absorption in silicene molecules. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 7387-7390	7.1	7
18	Plasmon coupling behavior in aluminium nanoparticle arrangements. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 10616-10619	7.1	3
17	Optical properties of Al nanostructures from time dependent density functional theory. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 134305	3.9	4
16	Computational Study of Magic-Size CdSe Clusters with Complementary Passivation by Carboxylic and Amine Ligands. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 10015-10019	3.8	28
15	Absorption Spectra of CuGaSe <sub>2</sub> and CuInSe <sub>2</sub> Semiconducting Nanoclusters. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 22732-22736	3.8	4
14	Gd doped Au nanoclusters: Molecular magnets with novel properties. <i>Chemical Physics Letters</i> , <b>2014</b> , 592, 217-221	2.5	4
13	Magnetism, structure and chemical order in small CoPd clusters: A first-principles study. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2014</b> , 349, 109-115	2.8	11
12	Structural and Optical Properties of Si-Doped Ag Clusters. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 4885-4889	3.8	9
11	Magnetic Phase Transition in 2 nm Ni <sub>x</sub> Cu <sub>1-x</sub> (0 ≤ x ≤ 1) Clusters. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 8169-8173	3.8	4
10	Tuning the optical response in carbon doped boron nitride nanodots. <i>Journal of Materials Chemistry C</i> , <b>2014</b> , 2, 8322-8327	7.1	12
9	Catalytically favorable surface patterns in Pt@Au nanoclusters. <i>RSC Advances</i> , <b>2013</b> , 3, 15350	3.7	7
8	Exotic High Activity Surface Patterns in Pt@Au Nanoclusters. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 9275-9280	3.8	9

7	Nanometer size 3d $\bar{A}$ d and 3d $\bar{B}$ d substitutional clusters: Promising candidates for magnetic storage applications. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2013</b> , 334, 31-35	2.8	5
6	Tuning the chemical activity through PtAu nanoalloying: a first principles study. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 9885	13	15
5	Photoabsorption Spectra of (Mo/W)@Au <sub>12</sub> Si <sub>60</sub> Clusters from Time-Dependent DFT Calculations. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 23938-23941	3.8	7
4	First-principles study of structural, magnetic, and electronic properties of small Fe-Rh alloy clusters. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	36
3	Interplay between Chemical and Magnetic Order in FeRh Clusters. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 17228-17238	3.8	22
2	Shapes matter: examining the optical response evolution in stretched aluminium nanoparticles via time-dependent density functional theory		1
1	One-dimensional aluminum nanoparticle chains: the influence of interparticle spacing and chain length on plasmon coupling behavior		1