
Author details

Faculty Name	Randhir Singh
Designation	Assistant Professor (Physics)
Qualification	PhD
Research field(s):	Molecular modelling Density functional theory Computational chemistry Vibrational spectroscopy
Journal publications =	5
Conference papers =	2
Total publications =	7
PhD thesis link:	http://hdl.handle.net/10603/235205
Online profile IDs:	
Vidwan ID	151696
Google scholar ID	6fj4_rEAAAAAJ&hl=en
Researchgate ID	Randhir_Singh14
Scopus ID	56949348300
WoS/Publons ID	N-5744-2015
ORCID ID	0000-0002-2820-8546
YouTube Channel ID:	physicslecturesbydrandhirsingh

Table 1: Author Details

Summary of Publications

Title	Year	Details
Experimental and Theoretical Vibrational Spectroscopic Analysis of Etoricoxib	2020	Details at S. No. 1
Effect of Pyridine on the Structure and Vibrations of Cobalt Phthalocyanine	2020	Details at S. No. 2
Effect of asymmetrical peripheral substitution of sulfonic acid group on the geometric and electronic structures and vibrations of copper phthalocyanine studied by computational and experimental techniques	2019	Details at S. No. 3
Computational study of effect of solvents on vibrational spectra of coumarin 500	2018	Details at S. No. 4

Solvation of coumarin6 studied by vibrational spectroscopy and density functional theory	2016	Details at S. No. 5
Computational study of charge transfer interactions in coumarin 480 using density functional theory	2018	Details at S. No. 6
Solvation of coumarin 500 studied by vibrational spectroscopy and density functional theory	2011	Details at S. No. 7

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Journal Publications

1 Experimental and Theoretical Vibrational Spectroscopic Analysis of Etoricoxib

Journal or Conference	Journal paper
Journal name	Materials today: Proceedings (Elsevier)
National/International	International
Whether Refereed (Peer Reviewed)	Yes
SCI/SCIE/Scopus	Scopus
ISBN/ ISSN/ Accn No.	2214-7853
Source Normalized Impact factor (Thomson Reuters)	0.694 (at the time of publication)
First author	Ritika Sachdeva
Co-authors	Prabhjot Kaur, Abhinav Soni, Randhir Singh, Vasant Sathe, V. P. Singh, G. S. S. Saini
Corresponding author	G. S. S. Saini
Year	Feb 2020 (online)
Volume	21
Issue	4
Page No.	1981-1990
DOI (if applicable)	https://doi.org/10.1016/j.matpr.2020.01.315
URL	https://www.sciencedirect.com/science/article/pii/S2214785320304028

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2 Effect of Pyridine on the Structure and Vibrations of Cobalt Phthalocyanine

Journal or Conference	Journal paper
Journal name	Materials today: Proceedings (Elsevier)
National/International	International
Whether Refereed (Peer Reviewed)	Yes
SCI/SCIE/Scopus	Scopus
ISBN/ ISSN/ Accn No.	2214-7853
Source Normalized Impact factor (Thomson Reuters)	0.694 (at the time of publication)

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Table 4 – continued from previous page

First author	Prabhjot Kaur
Co-authors	Sukh Dev Dogra, Ritika Sachdeva, Randhir Singh, Sukhwinder Singh, S.K. Tripathi, G. S. S. Saini
Corresponding author	Prabhjot Kaur
Year	Feb 2020 (online)
Volume	21
Issue	4
Page No.	1809-1817
DOI (if applicable)	https://doi.org/10.1016/j.matpr.2020.01.235
URL	https://www.sciencedirect.com/science/article/pii/S2214785320303011

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3 Effect of asymmetrical peripheral substitution of sulfonic acid group on the geometric and electronic structures and vibrations of copper phthalocyanine studied by computational and experimental techniques

Journal or Conference	Journal paper
Journal name	Journal of molecular structure (Elsevier)
National/International	International
Whether Refereed (Peer Reviewed)	Yes
SCI/SCIE/Scopus	SCIE + Scopus
ISBN/ ISSN/ Accn No.	0022–2860
Impact factor (Thomson Reuters)	2.011 (at the time of publication)
First author	Prabhjot Kaur
Co-authors	Ritika Sachdeva, Randhir Singh, Nazilla Soleimanioum, Sukhwinder Singh, G. S. S. Saini
Corresponding author	Prabhjot Kaur
Year	July 2018 (online), Jan 2019 (print)
Volume	1175
Issue	C
Page No.	314-334
DOI (if applicable)	https://doi.org/10.1016/j.molstruc.2018.07.082
URL	https://www.sciencedirect.com/science/article/abs/pii/S0022286018309013

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4 Computational study of effect of solvents on vibrational spectra of coumarin 500

Journal or Conference	Journal paper
Journal name	Computational and theoretical chemistry (Elsevier)
National/International	International
Whether Refereed (Peer Reviewed)	Yes
SCI/SCIE/Scopus	SCI + Scopus
ISBN/ ISSN/ Accn No.	2210-271X
Impact factor (Thomson Reuters)	1.549 (at the time of publication)
First author	Randhir Singh
Co-authors	Prabhjot Kaur, Ritika Sachdeva, J. S. Grewal,

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Table 6 – continued from previous page

Corresponding author	Vasant Sathe, G. S. S. Saini
Year	Randhir Singh
Volume	2018
Issue	1130
Page No.	C
DOI (if applicable)	46-57
URL	https://doi.org/10.1016/j.comptc.2018.03.008
	https://www.sciencedirect.com/science/article/pii/S2210271X18300902

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5 Solvation of coumarin6 studied by vibrational spectroscopy and density functional theory

Journal or Conference	Journal paper
Journal name	Journal of molecular structure (Elsevier)
National/International	International
Whether Refereed (Peer Reviewed)	Yes
SCI/SCIE/Scopus	SCIE + Scopus
ISBN/ ISSN/ Accn No.	0022–2860
Impact factor (Thomson Reuters)	1.753 (at the time of publication)
First author	Randhir Singh
Co-authors	Vasant Sathe, Amit Sharma, Sarvpreet Kaur, G. S. S. Saini
Corresponding author	Randhir Singh
Year	2016
Volume	1106
Issue	C
Page No.	170-180
DOI (if applicable)	https://doi.org/10.1016/j.molstruc.2015.10.073
URL	https://www.sciencedirect.com/science/article/abs/pii/S0022286015303732

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Conference Publications

6 Computational study of charge transfer interactions in coumarin 480 using density functional theory

Journal or Conference	Conference paper
Conference Name	International symposium on functional materials: (ISFM-2018) Energy and biomedical applications, Chandigarh
Dates	13-15 Apr., 2018
National/International	International
Organised by	IIT Kanpur, P. U. Chandigarh and University of Illinois, Chicago
SCI/SCIE/Scopus	NA
ISBN/ ISSN/ Accn No.	NA
First author	Randhir Singh
Co-authors	J. S. Grewal, Prabhjot Kaur, Ritika Sachdeva, G. S. S. Saini
Corresponding author	Randhir Singh
Paper ID	P-74
Page No.	110 (conference proceedings booklet)

7 Solvation of coumarin 500 studied by vibrational spectroscopy and density functional theory

Journal or Conference	Conference paper
Conference Name	International conference on advances in condensed and nanomaterial (ICACNM-2011), Chandigarh
Dates	23-26 Feb., 2011
National/International	International
Organised by	Department of Physics, P. U. Chandigarh
SCI/SCIE/Scopus	NA
ISBN/ ISSN/ Accn No.	NA
First author	G. S. S. Saini
Co-authors	Sarvpreet Kaur, Randhir Singh
Corresponding author	Randhir Singh
Year	2011
Paper ID	PAP No. P-217, PP-204
Page No.	163 (conference proceedings booklet)
