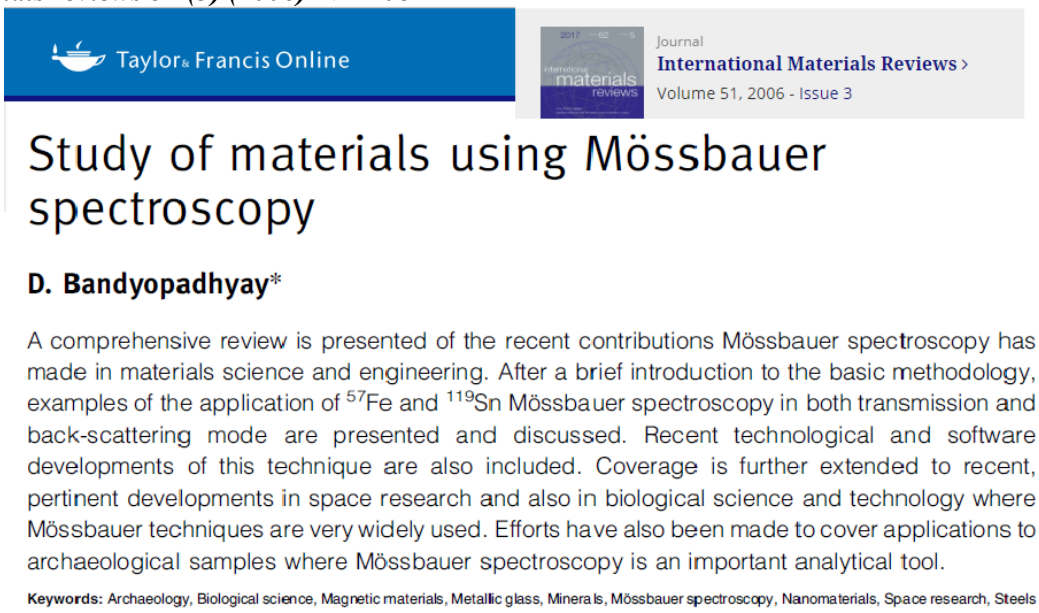
LIST OF PUBLICATIONS

Sl.No	***Publication details***	***IF***
	Focus: Single authorship Invited review article with IF 16.8 ***Study of materials using Mössbauer spectroscopy, Debashis Bandyopadhyay, International materials reviews 51 (3) (2006) 171-208*** 	***2006 IF 16.8***
64	*Unveiling reversible hydrogen storage mechanism on transition metal decorated 2D holey graphyne: A density functional study, Chaithanya Purushottam Bhat, Breeti Bandyopadhyay, Debashis Bandyopadhyay, International Journal of Hydrogen Energy 148 (2025) 150044, https://doi.org/10.1016/j.ijhydene.2025.150044*	***2025 IF 8.3***

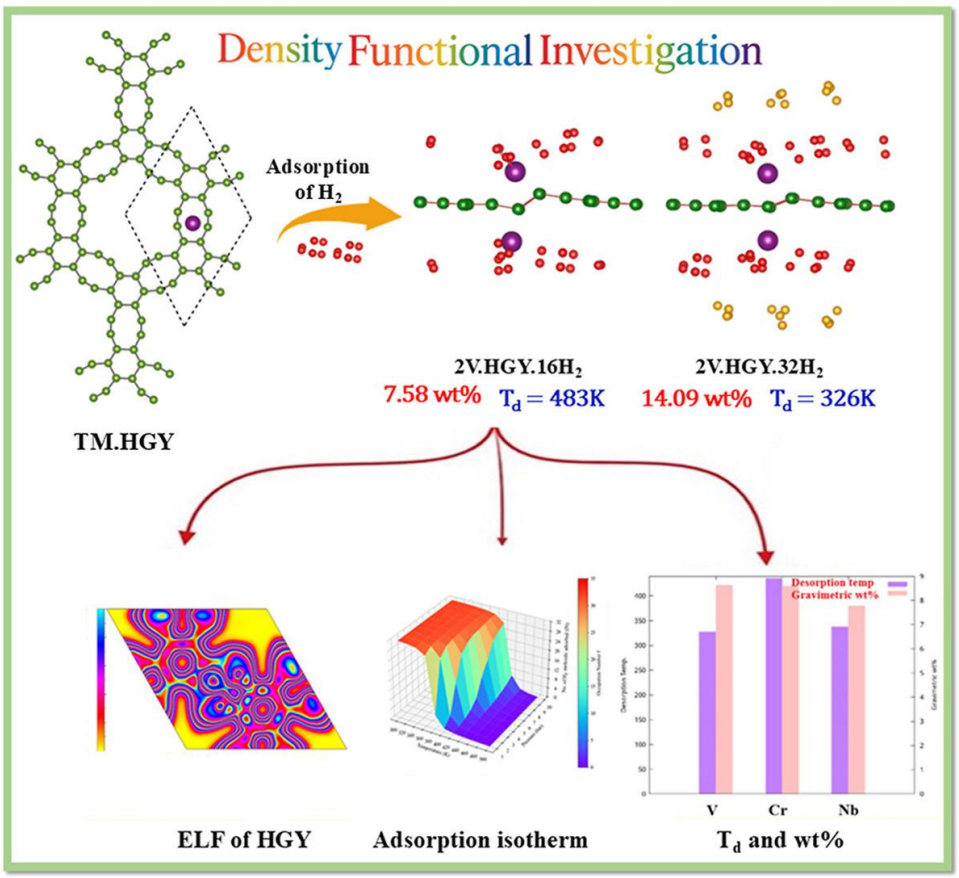
International Journal of Hydrogen Energy
Volume 148, 16 July 2025, 150044

Unveiling reversible hydrogen storage mechanism on transition metal decorated 2D holey graphyne: A density functional study

Chaithanya Purushottam Bhat [a], Breeti Bandyopadhyay [b], Debashis Bandyopadhyay [a]

https://doi.org/10.1016/j.ijhydene.2025.150044

Graphical abstract



63	*Insights into the reversible hydrogen storage mechanism of transition metal-decorated Irida-graphene: A DFT study, Chithanya Purushottam Bhat, Debashis Bandyopadhyay, International Journal of Hydrogen Energy 137(2025) 750-761* *https://doi.org/10.1016/j.ijhydene.2025.05.072*	***2025 IF 8.3***

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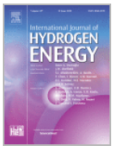
International Journal of Hydrogen Energy

Volume 137, 12 June 2025, Pages 750-761



Insights into the reversible hydrogen storage mechanism of transition metal-decorated Irida-graphene: A DFT study

Chaithanya Purushottam Bhat, Debashis Bandyopadhyay

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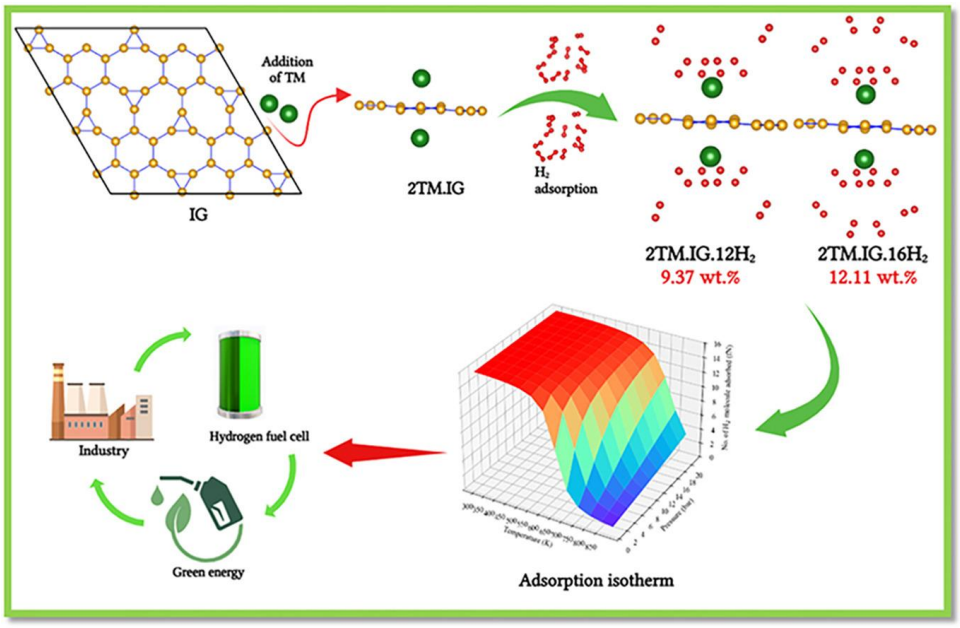

62	*A Novel 2D-hBNX Covalent Inorganic Framework Functionalized with Transition Metals for Enhanced Catechol Sensing: A Density Functional Investigation* *Chaithanya Purushottam Bhat, Debashis Bandyopadhyay, Surfaces and Interfaces 67 (2025) 106653,*	***2025 IF 6.7***

Surfaces and Interfaces
Volume 67, 15 June 2025, 106653

A Novel 2D-*h*BNX covalent inorganic framework functionalized with transition metals for enhanced catechol sensing: A density functional investigation

Chaithanya Purushottam Bhat, Debashis Bandyopadhyay

https://doi.org/10.1016/j.surfin.2025.106653

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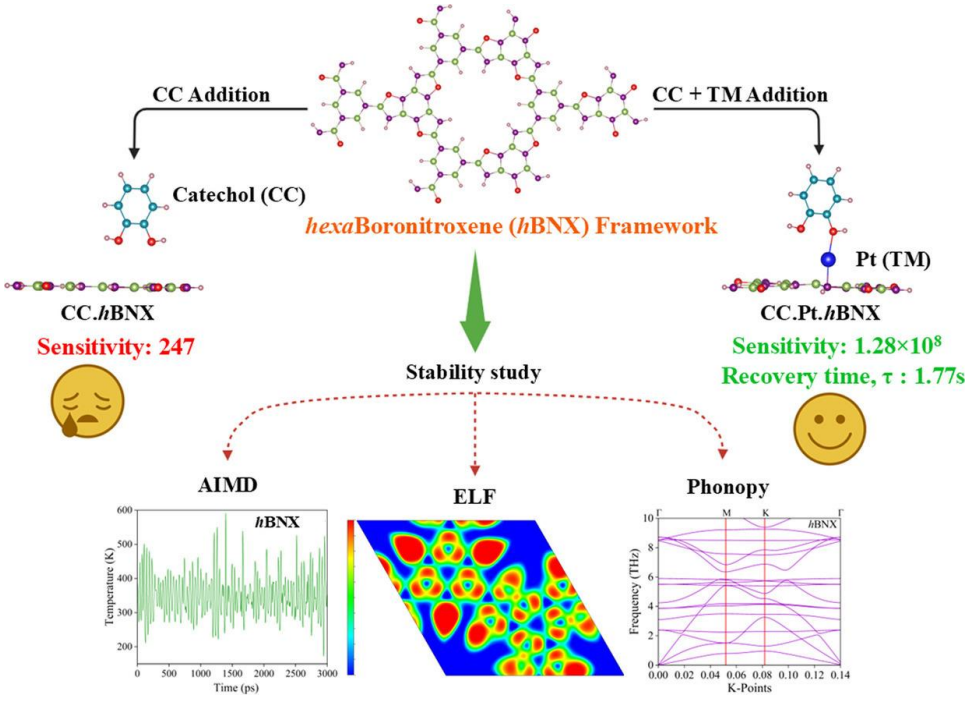


61	*Insights of Ti-doping on the hydrogen adsorption properties of the 2D-BeN4 monolayer: A density functional investigation, CP Bhat, D Bandyopadhyay International Journal of Hydrogen Energy 102 (2025) 1168-1179*	***2025 IF 8.3***

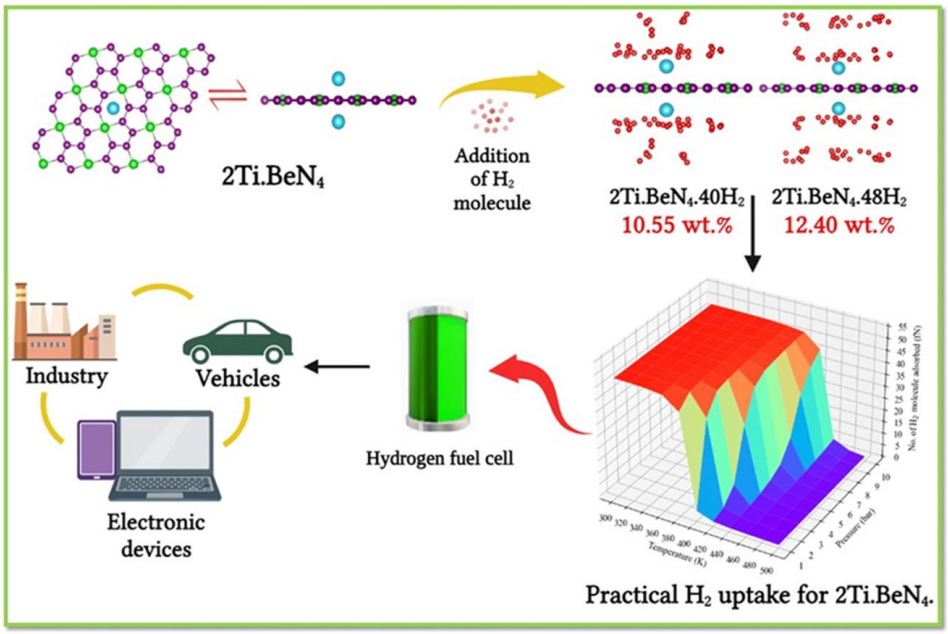
International Journal of Hydrogen Energy
Volume 102, 10 February 2025, Pages 1168-1179

Insights of Ti-doping on the hydrogen adsorption properties of the 2D-BeN_4 monolayer: A density functional investigation

Chaithanya Purushottam Bhat, Debashis Bandyopadhyay

https://doi.org/10.1016/j.ijhydene.2025.01.139

Graphical abstract



60	*Investigating the stable structures of yttrium oxide clusters: Y_n clusters as promising candidates for O_2 dissociation, Varun Vinayak Deshpande, Debashis Bandyopadhyay, Vaibhav Chauhan, Gayatri Kumari, Soumen Bhattacharyya, Dalton Transactions 54 (16), (2025) 6402-6410,*	***2025 IF 3.5***

Issue 16, 2025

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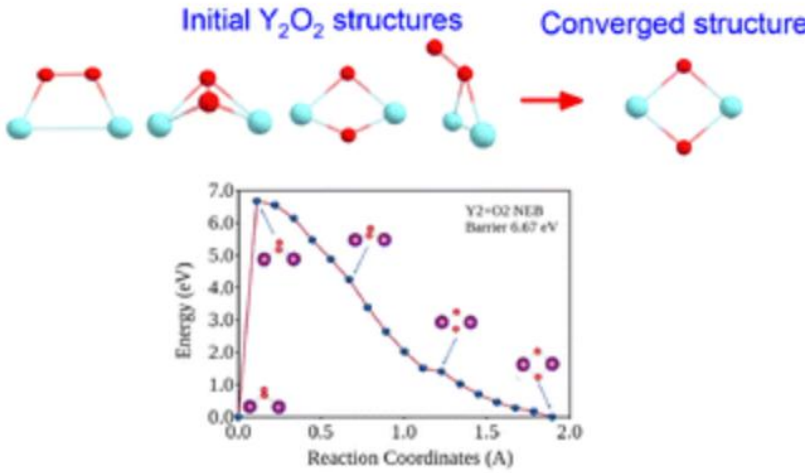
From the journal:
Dalton Transactions

Investigating the stable structures of yttrium oxide clusters: Y_n clusters as promising candidates for O_2 dissociation†

Varun Vinayak Deshpande,[ab] Debashis Bandyopadhyay,[c] Vaibhav Chauhan,[a] Gayatri Kumari[a] and Soumen Bhattacharyya[*ab]



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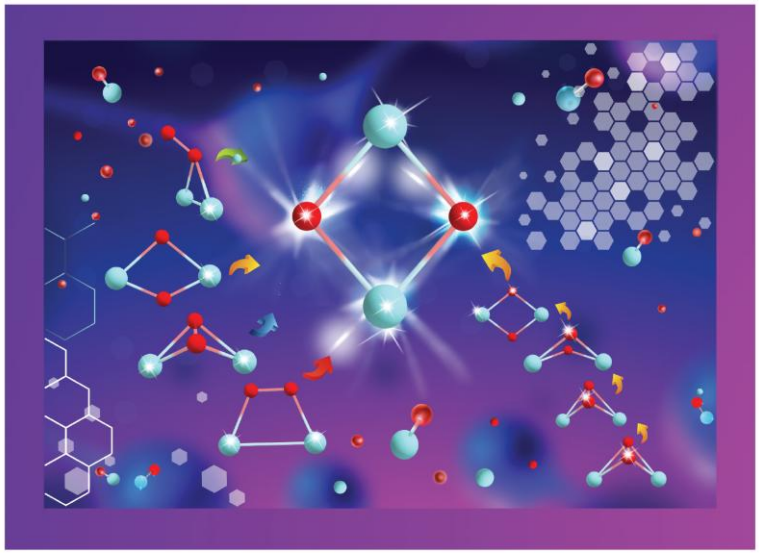

59

Hydrogen storage in Ti doped 4-6-8 biphenylene (Ti. C468): Insights from density functional theory, Chaithanya Purushottam Bhat, Debashis Bandyopadhyay
International Journal of Hydrogen Energy 79 (2025) 377-393,
https://doi.org/10.1016/j.ijhydene.2024.06.335

2025 IF 8.3

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International Journal of Hydrogen Energy

Volume 79, 19 August 2024, Pages 377-393

Hydrogen storage in Ti doped 4-6-8 biphenylene (Ti.C468): Insights from density functional theory

Chaithanya P. Bhat, Debashis Bandyopadhyay

https://doi.org/10.1016/j.ijhydene.2024.06.335

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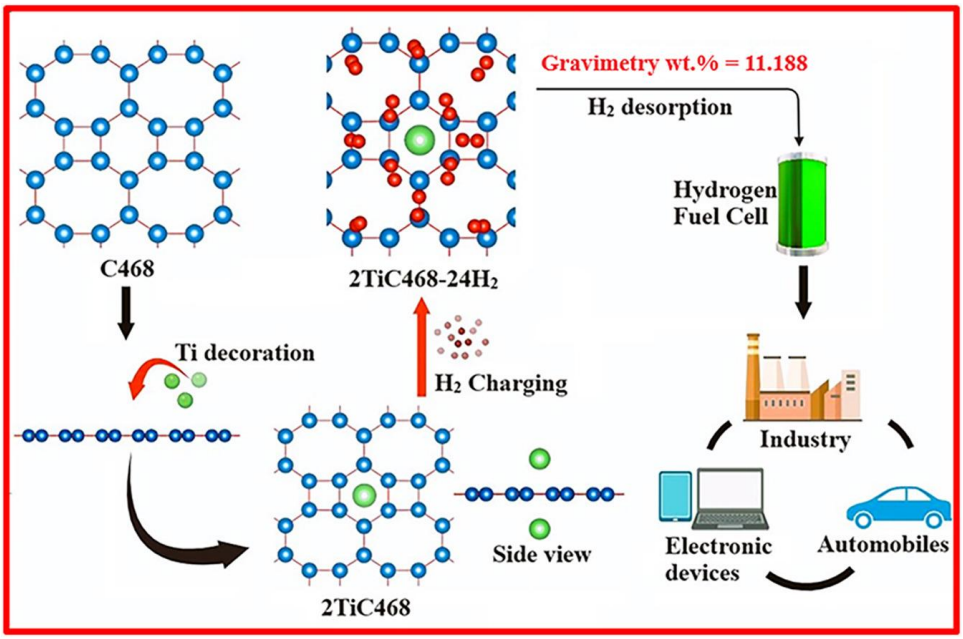

58

Hydrogen storage on MgO supported TiMgn (n= 2–6) clusters: A first principle investigation, S Chatterjee, D Bandyopadhyay, International Journal of Hydrogen Energy 77, (2024) 1467-1475,

2024 IF 8.3

International Journal of Hydrogen Energy
Volume 77, 5 August 2024, Pages 1467-1475

Hydrogen storage on MgO supported $TiMg_n$ (n=2–6) clusters: A first principle investigation

Soham Chatterjee, Debashis Bandyopadhyay

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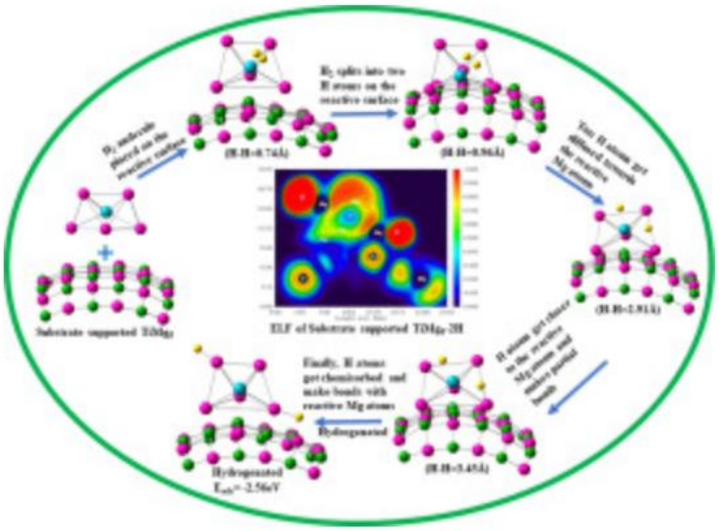
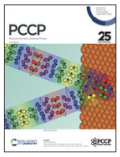
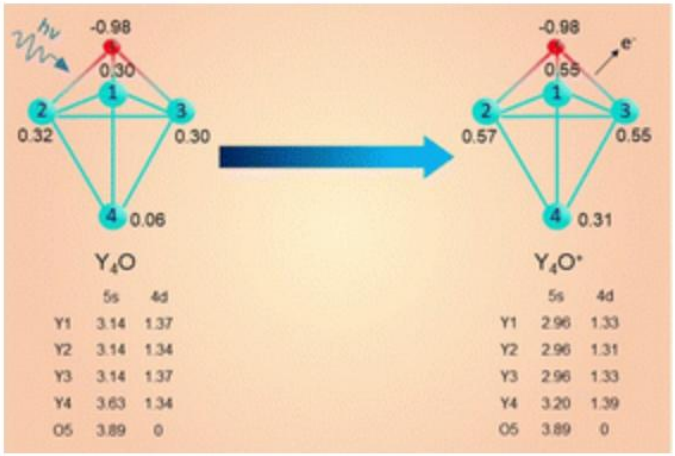
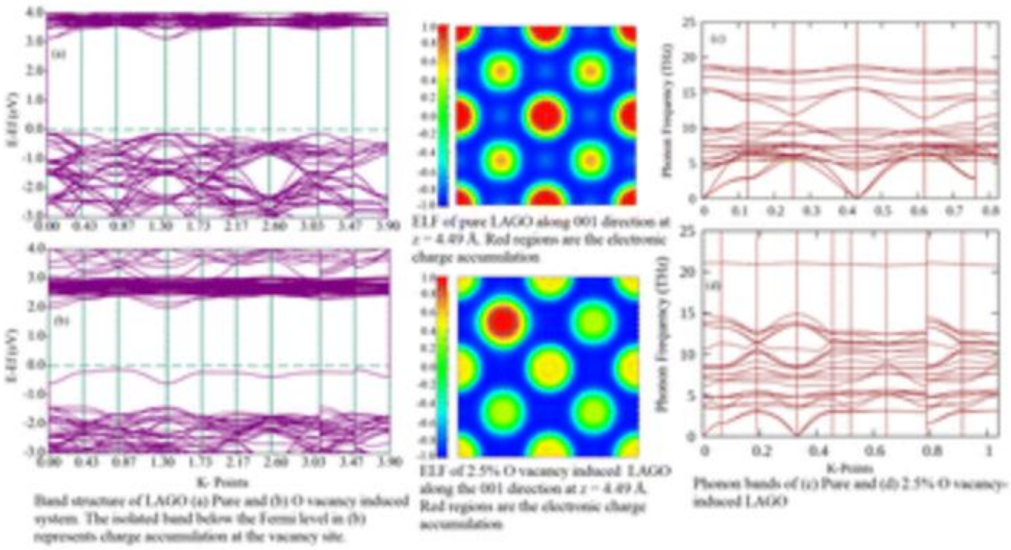


57	*Structure of small yttrium monoxide clusters, chemical bonding, and photoionization: threshold photoionization and density functional theory investigations, Varun Vinayak Deshpande, Vaibhav Chauhan, Debashis Bandyopadhyay, Anakuthil Anoop, Soumen Bhattacharyya,* ***Phys. Chem. Chem. Phys.****, 2024,****26****, 20123-20133 https://doi.org/10.1039/D4CP02351J*	***2024 IF 3.67***

	Issue 29, 2024 Previous Article Next Article  From the journal: Physical Chemistry Chemical Physics **Structure of small yttrium monoxide clusters, chemical bonding, and photoionization: threshold photoionization and density functional theory investigations†** Check for updates Varun Vinayak Deshpande,[ab] Vaibhav Chauhan,[a] Debashis Bandyopadhyay,[c] Anakuthil Anoop[d] and Soumen Bhattacharyya[*ab]  	
56	*The role of oxygen defects in the electronic, optical and phonon dispersion of the LAGO perovskite: a density functional theory investigation,Chaithanya Purushottam Bhat, Ashwin K Godbole, Debashis Bandyopadhyay,* ***Dalton Trans.****, 2023,****52****, 16128-16139, DOI: 10.1039/d3dt02846a*	***2023 IF 3.5***

	Issue 44, 2023 Previous Article | Next Article  From the journal: **Dalton Transactions** **The role of oxygen defects in the electronic, optical and phonon dispersion of the LAGO perovskite: a density functional theory investigation** † Check for updates Chaithanya P. Bhat,[a] Ashwin K. Godbole[a] and Debashis Bandyopadhyay *[a]  Band structure of LAGO (a) Pure and (b) O vacancy induced system. The isolated band below the Fermi level in (b) represents charge accumulation at the vacancy site. ELF of pure LAGO along 001 direction at $z = 4.49$ Å. Red regions are the electronic charge accumulation ELF of 2.5% O vacancy induced LAGO along the 001 direction at $z = 4.49$ Å. Red regions are the electronic charge accumulation Phonon bands of (c) Pure and (d) 2.5% O vacancy-induced LAGO 5 2023	
55	*First Principle Study on the Electronic and Optical Properties of KTaO3 for Optoelectronic Properties, Trideeb Bhattacharya, Taha Yussuf Raja, Debashis Bandyopadhyay, 2023 IEEE Fifth International Conference on Advances in Electronics, Computers and Communications (ICAECC) (2023)* *Pages 01-04*	***2023***
54	*Ionization Energies and Ground-State Structures of Neutral Lan (n = 2–14) Clusters: A Combined Experimental and Theoretical Investigation* *S Bhattacharyya, D Bandyopadhyay, S Mukund, P Sen, SG Nakhate* *The Journal of Physical Chemistry A 126 (20),(2022) 3135-3144* *https://doi.org/10.1021/acs.jpca.2c00967*	***2022*** ***IF*** ***2.7***

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Ionization Energies and Ground-State Structures of Neutral La_n (n = 2–14) Clusters: A Combined Experimental and Theoretical Investigation

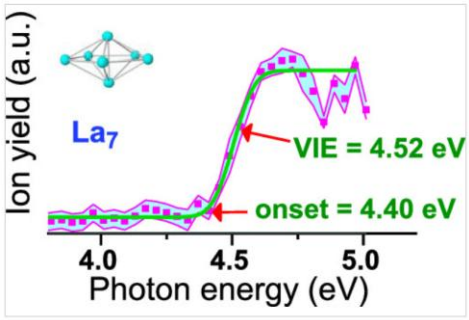
Soumen Bhattacharyya*, Debashis Bandyopadhyay, Sheo Mukund, Prasenjit Sen, and Sanjay G. Nakhate

Cite this: *J. Phys. Chem. A* 2022, 126, 20, 3135–3144
Publication Date: May 17, 2022
https://doi.org/10.1021/acs.jpca.2c00967

The Journal of Physical Chemistry A

Abstract

Neutral lanthanum clusters are studied by photoionization time-of-flight mass spectroscopy, laser threshold photoionization spectroscopy, and density functional theory (DFT). Mass abundance spectra (MS) registered at multiple photoionization wavelengths in the range of 195–230 nm by single photon ionization reveal the production of all sizes, La_n ($n \geq 50$), in good abundance, nullifying previously predicted low abundances for certain sizes in the 3–14 size range. Also, the MS do not reveal the extraordinary stability of any specific size, as one would expect, from previous theoretical predictions of 7- and 13-atom clusters as magic. Ionization energies (IEs) are measured for La_n (n = 2–14) clusters. DFT has been used to determine the stable geometric isomers for 2- to 10-atom clusters and to calculate their IEs. The theoretical IEs of 2–7 atom clusters are in decent agreement with their experimental values; however, the theoretical IEs are somewhat lower by ~0.4 eV for $n \geq 8$ than their experimental IEs.



53 | *Insights into the electronic structure and stability of TiMgn (n= 1–12) clusters: Validation of electron counting rule, S Chatterjee, D Bandyopadhyay, Materials Today Communications 32 (2022) 103860, https://doi.org/10.1016/j.mtcomm.2022.103860*

2022 IF 4.5

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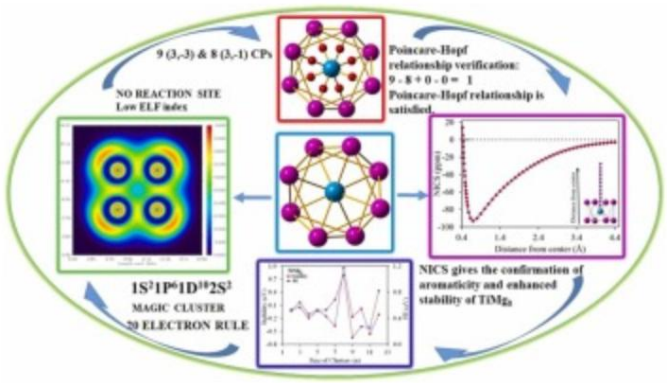
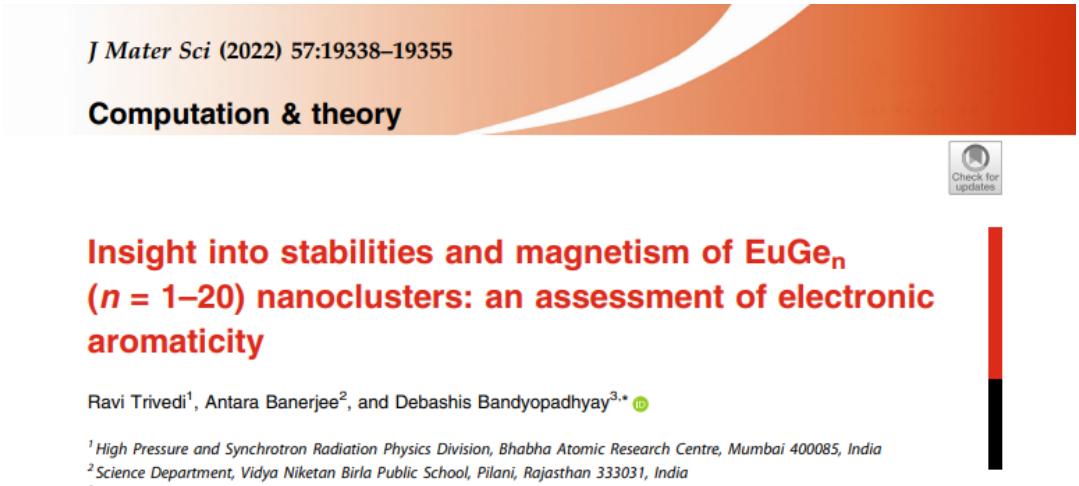
Volume 32, August 2022, 103860

Insights into the electronic structure and stability of $TiMg_n$ (n=1–12) clusters: Validation of electron counting rule

Soham Chatterjee, Debashis Bandyopadhyay

	Graphical Abstract 	
52	*Insight into stabilities and magnetism of EuGen (n = 1–20) nanoclusters: an assessment of electronic aromaticity, Journal of Materials Science, 57 (2022) 19338–19355, https://doi.org/10.1007/s10853-022-07834-0* 	***2022 IF 3.5***

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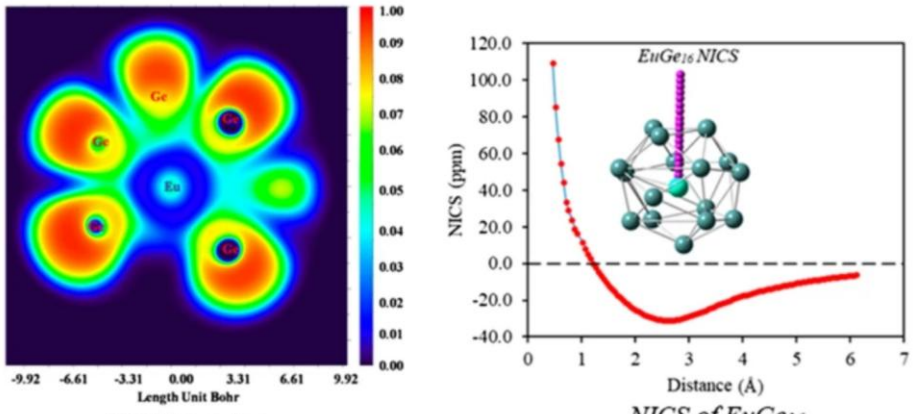

ELF Mapping *NICS of $EuGe_{16}$*

ELF mapping and NICS show the presence of strong aromaticity in $EuGe_{16}$. Among the top 34 electrons, 18σ and 16π electrons (S.I.). The 18σ electrons follow Hirsch's $2(n+1)^2$ σ-electron rule for n=2. The remaining 16π electrons do not directly follow Hückel's (4n+2) π–electron rule. Splitting it as 6π + 10π satisfies Hückel's rule for n=1 and 2, respectively. So, by applying the mixed π-σ electron counting rule, the enhanced stability of the $EuGe_{16}$ cluster can explain.

51 *Insights into catalytic behavior of $TiMg_n$ (n=1-12) nanoclusters in hydrogen storage and dissociation process: A DFT investigation,* ***Debashis Bandyopadhyay****, Soham Chatterjee, Ravi Trivedi, and Kapil Dhaka, Int. J. Hydrogen Energy, 47(2022)* 13418-13429, *(Online first), https://doi.org/10.1016/j.ijhydene.2022.02.091*

2022 IF 8.3

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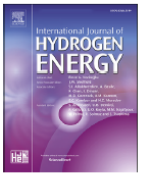
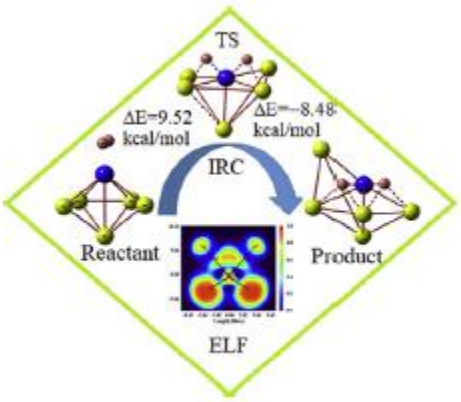


Insights into catalytic behavior of $TiMg_n$ (n=1–12) nanoclusters in hydrogen storage and dissociation process: A DFT investigation

Debashis Bandyopadhyay [a,*], Soham Chatterjee [a], Ravi Trivedi [b], Kapil Dhaka [c]

[a] Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan, 333031, India
[b] Department of Physics, Indian Institute of Technology, Powai, Mumbai, 400076, India
[c] Department of Materials Science and Engineering, Technion Israel Institute of Technology, Haifa, 3200003, Israel



50	*Study of electronic structure, stabilities and electron localization behavior of AgPbn (n= 1–14) nanoclusters: A first principal investigation. R Trivedi, A Banerjee,* ***Debashis Bandyopadhyay****, Physica E: Low-dimensional Systems and Nanostructures 131, 114725,* https://doi.org/10.1016/j.physe.2021.114725	***2021 IF 2.9***

Physica E 131 (2021) 114725

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Physica E: Low-dimensional Systems and Nanostructures

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Study of electronic structure, stabilities and electron localization behavior of $AgPb_n$ (n=1–14) nanoclusters: A first principal investigation

Ravi Trivedi [a], Antara Banerjee [b], Debashis Bandyopadhyay [c,*]

[a] Department of Physics, Indian Institute of Technology, Bombay, Mumbai, 400076, India
[b] Science Department, Vidya Niketan Birla Public School Pilani, Rajasthan, 333031, India
[c] Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan, 333031, India

49	*Ionization energies and structures of small lanthanum oxide clusters $(La_2O_3)_n.LaO$ (n = 1-3), Soumen Bhattacharyya, Prasenjit Sen, Sheo Mukund, Suresh Yarlagadda,* ***Debashis Bandyopadhyay*** *and Sanjay G. Nakhate, Eur. Phys. J. D (2019) 73: 158 DOI: 10.1140/epjd/e2019-100185-5*	***2019 IF 1.5***

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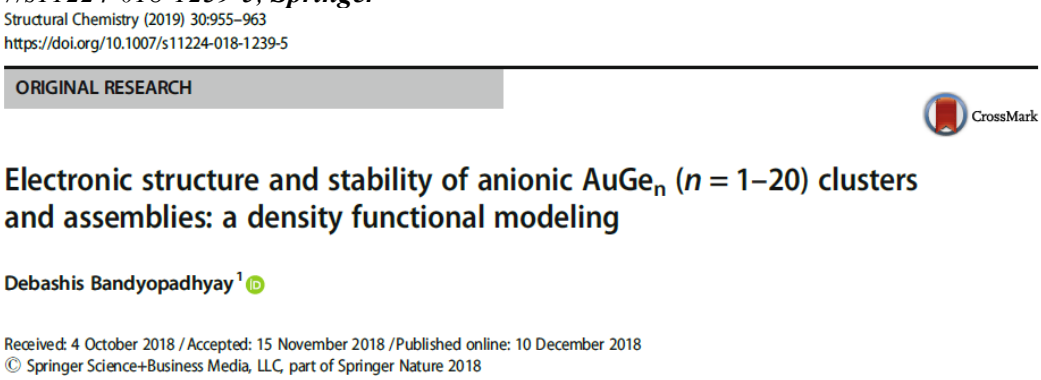
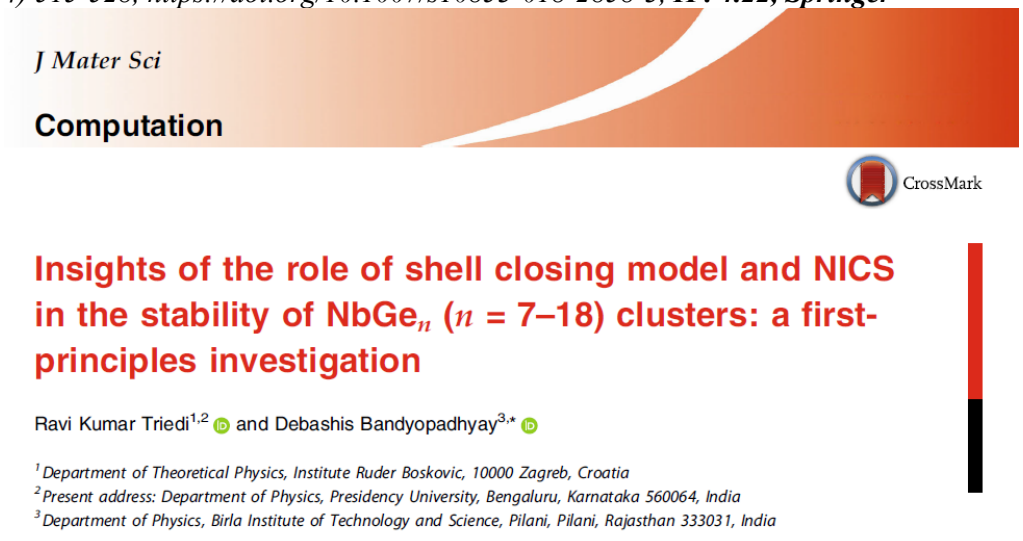
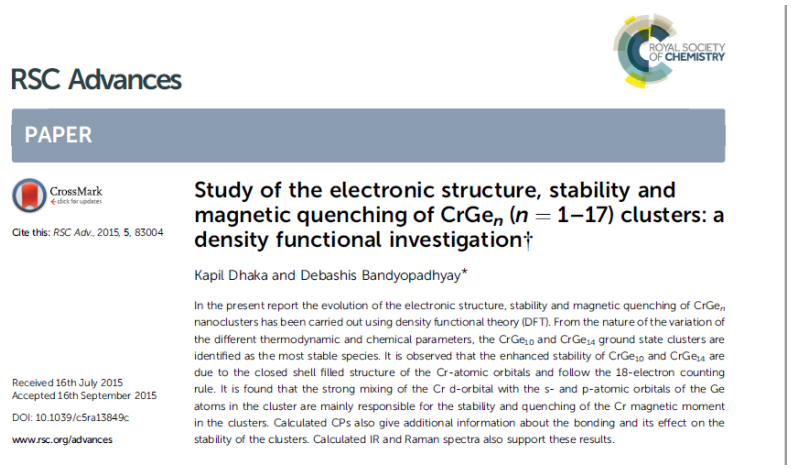
Eur. Phys. J. D (2019) 73: 158 DOI: 10.1140/epjd/e2019-100185-5

Ionization energies and structures of small lanthanum oxide clusters $(La_2O_3)_n.LaO$ $(n = 1–3)$

Soumen Bhattacharyya, Prasenjit Sen, Sheo Mukund, Suresh Yarlagadda, Debashis Bandyopadhyay, and Sanjay G. Nakhate

48	*Electronic structure and stability of anionic $AuGe_n$ (n=1-20) clusters and assemblies: A density functional modelling,* ***Debashis Bandyopadhyay****, Structural Chemistry, (2019) 30: 955-963, DOI: 10.1007/s11224-018-1239-5,* ***Springer***  Structural Chemistry (2019) 30:955–963 https://doi.org/10.1007/s11224-018-1239-5 ORIGINAL RESEARCH CrossMark **Electronic structure and stability of anionic $AuGe_n$ (n = 1–20) clusters and assemblies: a density functional modeling** Debashis Bandyopadhyay[1] Received: 4 October 2018 / Accepted: 15 November 2018 / Published online: 10 December 2018 © Springer Science+Business Media, LLC, part of Springer Nature 2018	***2019 IF 2.1***
47	*Insights of the role of shell closing model and NICS in the stability of $NbGe_n$ (n = 7-18) clusters: A first principle investigation, Ravi Trivedi and* ***Debashis Bandyopadhyay****, Journal of Materials Science, 2019 (54) 515-528, https://doi.org/10.1007/s10853-018-2858-3,* ***IF. 4.22, Springer***  *J Mater Sci* **Computation** CrossMark **Insights of the role of shell closing model and NICS in the stability of $NbGe_n$ (n = 7–18) clusters: a first-principles investigation** Ravi Kumar Triedi[1,2] and Debashis Bandyopadhyay[3,*] [1] Department of Theoretical Physics, Institute Ruder Boskovic, 10000 Zagreb, Croatia [2] Present address: Department of Physics, Presidency University, Bengaluru, Karnataka 560064, India [3] Department of Physics, Birla Institute of Technology and Science, Pilani, Pilani, Rajasthan 333031, India	***2019 IF 3.5***
46	*Evolution of electronic and vibrational properties of $M@X_n$ (M = Ag, Au, X = Ge, Si, n=10, 12, 14) clusters: a density functional modeling, Ravi Trivedi and* ***Debashis Bandyopadhyay****, Journal of Materials Science, 53 (2018) 8263–8273, https://doi.org/10.1007/s10853-018-2002-4,* ***IF. 4.22****,* ***Springer***	***2018 IF 3.5***

	J Mater Sci (2018) 53:8263–8273 **Computation** CrossMark **Evolution of electronic and vibrational properties of $M@X_n$ (M = Ag, Au, X = Ge, Si, n = 10, 12, 14) clusters: a density functional modeling** Ravi Trivedi[1,*] and Debashis Bandyopadhyay[2] [1] Department of Theoretical Physics, Institute Ruder Boskovic, 10000 Zagreb, Croatia [2] Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan 333031, India	
45	*Study of adsorption and dissociation of H2 molecule on RgnRh (n=1-10) clusters: A first principle investigation*, Ravi Kumar Trivedi and ***Debashis Bandyopadhyay***, *International Journal of Hydrogen Energy, 41 (2016) 20113-20121, DOI: 10.1016/j.ijhydene.2016.09.007.* INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 41 (2016) 20113–20121 ELSEVIER Available online at www.sciencedirect.com ScienceDirect journal homepage: www.elsevier.com/locate/he **Study of adsorption and dissociation pathway of H_2 molecule on Mg_nRh (n = 1–10) clusters: A first principle investigation** CrossMark Ravi Trivedi, Debashis Bandyopadhyay* Department of Physics, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, 333031, India	**2016**
44	*Magnetism, structures and stabilities of cluster assembled TM@Si_n nanotubes (TM=Cr, Mn and Fe): A density functional study*, Kapil Dhaka and ***Debashis Bandyopadhyay***, *Dalton transactions, 45 (2016) 12432-12443, DOI: 10.1039/C6DTO1252C* Dalton Transactions ROYAL SOCIETY OF CHEMISTRY PAPER Magnetism, structures and stabilities of cluster assembled TM@Si nanotubes (TM = Cr, Mn and Fe): a density functional study† Kapil Dhaka and Debashis Bandyopadhyay* Introduction	**2016** **IF** **3.5**

43	*Study of electronic structure, stability and magnetic quenching of $CrGe_n$ (n=1-17) clusters: A density functional investigation, Kapil Dhaka,* ***Debashis Bandyopadhyay****, RSC Advances, 15 (2015) 83004-83012, DOI: 10.1039/C5RA13849C*  RSC Advances PAPER CrossMark Cite this: *RSC Adv.*, 2015, 5, 83004 Study of the electronic structure, stability and magnetic quenching of $CrGe_n$ ($n = 1–17$) clusters: a density functional investigation† Kapil Dhaka and Debashis Bandyopadhyay* In the present report the evolution of the electronic structure, stability and magnetic quenching of $CrGe_n$ nanoclusters has been carried out using density functional theory (DFT). From the nature of the variation of the different thermodynamic and chemical parameters, the $CrGe_{10}$ and $CrGe_{14}$ ground state clusters are identified as the most stable species. It is observed that the enhanced stability of $CrGe_{10}$ and $CrGe_{14}$ are due to the closed shell filled structure of the Cr-atomic orbitals and follow the 18-electron counting rule. It is found that the strong mixing of the Cr d-orbital with the s- and p-atomic orbitals of the Ge atoms in the cluster are mainly responsible for the stability and quenching of the Cr magnetic moment in the clusters. Calculated CPs also give additional information about the bonding and its effect on the stability of the clusters. Calculated IR and Raman spectra also support these results. Received 16th July 2015 Accepted 16th September 2015 DOI: 10.1039/c5ra13849c www.rsc.org/advances	***2015 IF 4.6***
42	*Hydrogen storage in small size Mg_nCo clusters: A density functional study, Ravi Trivedi,* ***Debashis Bandyopadhyay****, International Journal of Hydrogen Energy, 40 (2015) 12727-12735, DOI: https://doi.org/10.1016/j.ijhydene.2015.07.122*  INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 40 (2015) 12727–12735 Available online at www.sciencedirect.com ScienceDirect journal homepage: www.elsevier.com/locate/he ELSEVIER Hydrogen storage in small size Mg_nCo clusters: A density functional study CrossMark Ravi Trivedi, Debashis Bandyopadhyay* Department of Physics, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, 333031, India	***2015 IF 8.3***
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	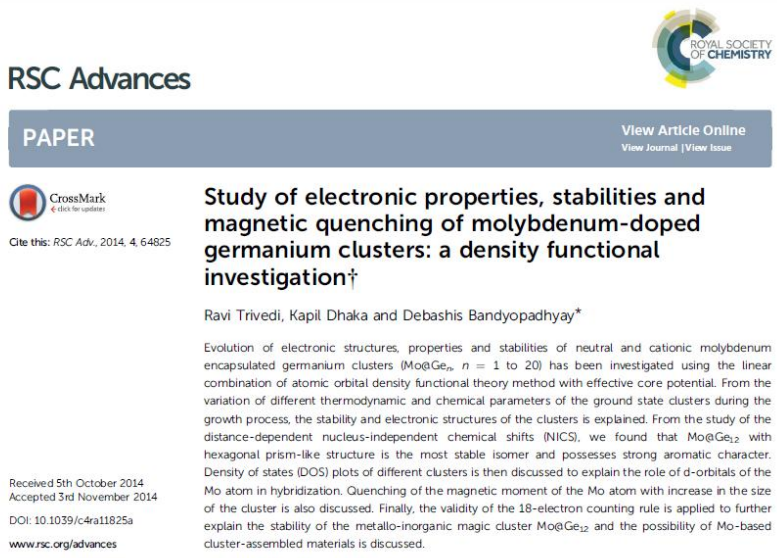	
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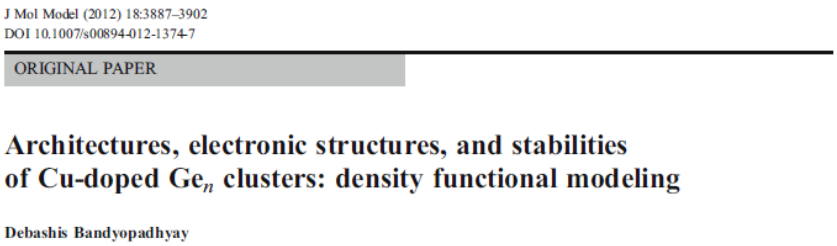
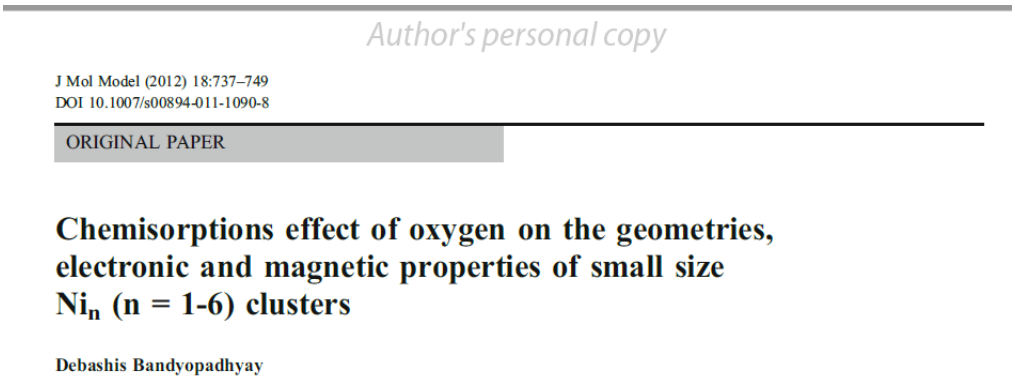
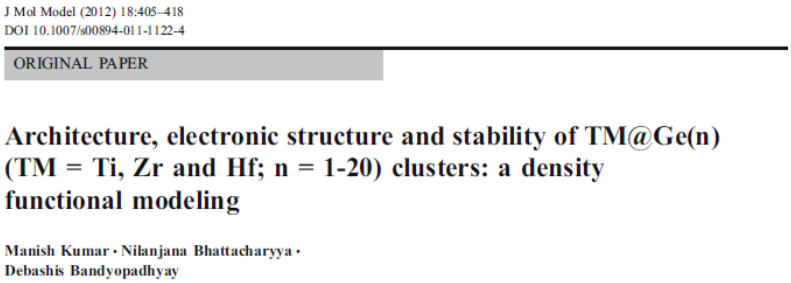
38	*Electronic structure and stabilities of Ni-doped germanium nanoclusters: a density functional modeling study, Kapil Dhaka, Ravi Trivedi,* ***Debashis Bandyopadhyay****, Journal of molecular modeling 19 (4) (2013) 1473-1488,* https://doi.org/10.1007/s00894-012-1690-y J Mol Model (2013) 19:1473–1488 DOI 10.1007/s00894-012-1690-y ORIGINAL PAPER **Electronic structure and stabilities of Ni-doped germanium nanoclusters: a density functional modeling study** **Kapil Dhaka · Ravi Trivedi · Debashis Bandyopadhyay**	***2013 IF 2.1***

37	*Architectures, electronic structures, and stabilities of Cu-doped Gen clusters: density functional modeling,* ***Debashis Bandyopadhyay****, Journal of molecular modeling 18 (8), (2012) 3887-3902* http://link.springer.com/article/10.1007/s00894-011-1090-8  J Mol Model (2012) 18:3887–3902 DOI 10.1007/s00894-012-1374-7 ORIGINAL PAPER **Architectures, electronic structures, and stabilities of Cu-doped Ge_n clusters: density functional modeling** Debashis Bandyopadhyay	***2012 IF 2.1***
36	*Chemisorptions effect of oxygen on the geometries, electronic and magnetic properties of small size Ni_n (n= 1-6) clusters,* ***Debashis Bandyopadhyay****, Journal of molecular modeling 18 (2012)737-749* https://doi.org/10.1007/s00894-011-1090-8,  Author's personal copy J Mol Model (2012) 18:737–749 DOI 10.1007/s00894-011-1090-8 ORIGINAL PAPER **Chemisorptions effect of oxygen on the geometries, electronic and magnetic properties of small size Ni_n (n = 1-6) clusters** Debashis Bandyopadhyay	***2012 IF 2.1***
35	*Architecture, electronic structure and stability of TM@Gen (TM= Ti, Zr and Hf; n= 1-20) clusters: a density functional modeling, Manis Kumar, Nilanjana Bhattacharyya,* ***Debashis Bandyopadhyay*** *Journal of Molecular Modeling 18 (2012) 405-418, https://doi.org/10.1007/s00894-011-1122-4*  J Mol Model (2012) 18:405–418 DOI 10.1007/s00894-011-1122-4 ORIGINAL PAPER **Architecture, electronic structure and stability of TM@Ge(n) (TM = Ti, Zr and Hf; n = 1-20) clusters: a density functional modeling** Manish Kumar · Nilanjana Bhattacharyya · Debashis Bandyopadhyay	***2012 IF 2.1***
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New Insights into Applicability of Electron-Counting Rules in Transition Metal Encapsulating Ge Cage Clusters

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The relative stability of Sc, Ti, and V encapsulating Ge_n clusters in the size range $n = 14-20$ has been studied through first-principles electronic structure calculations based on density functional theory. Variations of the embedding energy, gap between the highest occupied and the lowest occupied molecular orbitals, ionization potential, vertical detachment energy, and electron affinity with cluster size have been calculated to identify clusters with enhanced stability. The enhanced stability of some clusters can be very well explained as due to the formation of a filled shell free-electron gas inside the Ge cages. For the first time, direct evidence of the formation of a free-electron gas is also presented. In some other clusters, enhanced stability is found

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J. Phys. Chem. A **2010,** *114,* 1835–1842 **1835**

Density Functional Investigation of Structure and Stability of Ge_n and Ge_nNi ($n = 1-20$) Clusters: Validity of the Electron Counting Rule

Debashis Bandyopadhyay[†] and Prasenjit Sen[*,‡]

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Structure and electronic properties of neutral and cationic pure and Ni-doped Ge clusters containing 1−20 Ge atoms are calculated within the framework of linear combination of atomic orbitals density functional theory. It is found that in clusters containing more than 8 Ge atoms the Ni atom is absorbed endohedrally in the Ge cage. Relative stability of Ni-doped clusters at different sizes is studied by calculating their binding energy, embedding energy of a Ni atom in a Ge cluster, highest-occupied molecular orbital to lowest-unoccupied molecular orbital gap, and the second-order energy difference. Clusters having 20 valence electrons turn out to be relatively more stable in both the neutral and the cationic series. There is, infact, a sharp drop in IP as the valence electron count increases from 20 to 21, in agreement with predictions of shell models. Relevance of these results to the designing of Ge-based superatoms is discussed.

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Effect of Transition Metal Doping on Hydrog enated Germanium Nanocag es: A Density Functional Investigation

Debashis Bandyopadhyay[1,*], Manish Kumar[1], Bandhan Jot Singh[1,2], and Shantan Kajjam[1,2]

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In this report we present an ab initio electronic-str ucture calculations ofhydrogenated ger manium cages Ge_nH_nTM (TM = Cu and Zn, n= 12 to 24) using density functional theor y with polarized basis set (SDD) nanoclusters. In the first step of the calculation, geometr icaloptimizations of the nanoclustershave been done. In the next step only the ground state optimized geometr ies are used to calculate the binding energy(BE), HOMO-LUMO gap and embedding energy(EE)ofthe

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Density functional study of the electronic structure and properties of lithium intercalated graphite

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Abstract. Ab initio electronic-structure calculations are performed using density functional theory (DFT) with polarized basis set (LanL2DZ and 6-311G^{++}) within the spin polarized generalized gradient approximation for lithium intercalated graphite. Initially different benzene-Li^{+} model clusters are optimized on the basis of their total energy at room temperature. These model clusters are used to calculate the optimized structure of lithium intercalated graphite clusters. The resultant optimized structures are used to calculate dipole moment, ionization potential (IP), electron affinity (EA), binding energy (BE) and vibrational spectra (IR and Raman). For an idea of the band gap of the clusters in the ground state, the HOMO-LUMO gap (ΔE_g) has been calculated. To compare the electron transfer ability of different clusters, chemical potential (μ), hardness (η) and their ratio ($|\frac{\mu}{\eta}|$) for different clusters have also been

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Nanotechnology **20** (2009) 275202 (12pp) doi:10.1088/0957-4484/20/27/275202

Study of pure and doped hydrogenated germanium cages: a density functional investigation

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Abstract
In this paper we present an *ab initio* electronic-structure calculation performed using density functional theory (DFT) with a polarized basis set (SDD) within the spin polarized generalized gradient approximation for pure and divalent transition metal doped hydrogenated germanium nanocluster cages Ge_nH_nM (M = Zn, Cd and Hg, n = 6–28). In the first step of the calculation, geometrical optimizations of the nanoclusters are done. In the next step only the ground state optimized geometries are used to calculate the binding energy (E_b), HOMO–LUMO gap (ΔE_g) and embedding energy of the clusters. To study the optical behaviour of the clusters, IR

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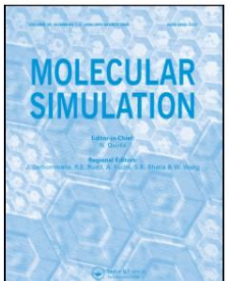

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The study of the electronic structures and properties of pure and transition metal-doped silicon nanoclusters: a density functional theory approach

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28	*The electronic structures and properties of transition metal-doped silicon nanoclusters: A density functional investigation,* ***Debashis Bandyopadhyay****, Manis Kumar, Chemical Physics 353 (1) (2008) 170-176, https://doi.org/10.1016/j.chemphys.2008.08.017*  Chemical Physics 353 (2008) 170–176 Contents lists available at ScienceDirect Chemical Physics journal homepage: www.elsevier.com/locate/chemphys The electronic structures and properties of transition metal-doped silicon nanoclusters: A density functional investigation Debashis Bandyopadhyay *, Manish Kumar Department of Physics, Birla Institute of Technology and Science, Pilani 333 031, Rajasthan, India ARTICLE INFO Article history: Received 4 April 2008 Accepted 20 August 2008 Available online 3 September 2008 Keywords: Ab initio DFT Nanoclusters Binding energy IR Raman IP EA ABSTRACT We report an ab initio all electron molecular-orbital electronic-structure calculation by using density functional theory (DFT) and with polarized basis set (LanL2DZ) within the spin polarized generalized gradient approximation for metal-doped silicon clusters, Si_nM (n = 14–20 and M = Ti, Zr, Hf). As the first step of calculation, geometrical optimizations of the nanoclusters have been done. In the next step, these optimized geometries are used to calculate the binding energy and HOMO–LUMO gap (band gap) of the clusters. In order to check the dynamical stability of the clusters, IR and Raman spectra have been calculated. Further calculations have been done on cation and anion clusters to obtain ionization potential (IP), electron affinity (EA), chemical potential and chemical hardness of the optimized clusters. © 2008 Elsevier B.V. All rights reserved.	***2008 IF 3.8***
27	*A density functional theory-based study of the electronic structures and properties of cage like metal doped silicon clusters,* ***Debashis Bandyopadhyay****, Journal of Applied Physics 104 (8) (2008) 4308, https://doi.org/10.1063/1.3000657* JOURNAL OF APPLIED PHYSICS **104**, 084308 (2008) **A density functional theory–based study of the electronic structures and properties of cage like metal doped silicon clusters** Debashis Bandyopadhyay[a)] *Department of Physics, Birla Institute of Technology and Science, Pilani Rajasthan 333031, India* (Received 29 August 2007; accepted 1 September 2008; published online 23 October 2008) *Ab initio* electronic-structure calculations were performed by using density functional theory with polarized basis set (LanL2DZ) within the spin polarized generalized gradient approximation for metal (M=Ti,Zr,Hf) doped Si_n clusters where n varies from 9 to 20. In the first step of the calculation, geometrical optimizations of the nanoclusters have been done. In the next step, these optimized geometries have been used to calculate the binding energy (BE) and HOMO-LUMO gap (ΔE_g) of the clusters. In order to check the stability of the clusters, the second order energy differences of the optimized geometries have been calculated. To study the optical behavior of the clusters, IR and Raman spectra calculation have been done. Further calculations on cation and anion clusters have been done to obtain their ionization potential (IP), electron affinity (EA), and chemical potential. © *2008 American Institute of Physics*. [DOI: 10.1063/1.3000657]	***2008 IF 2.7***
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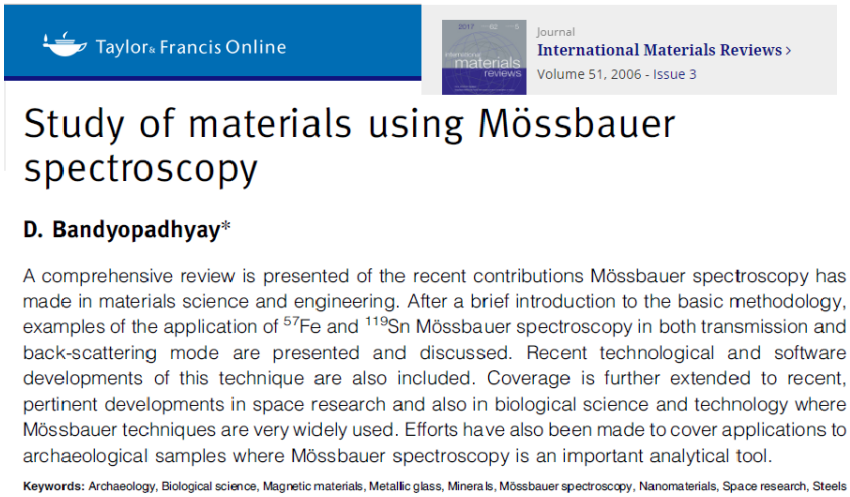
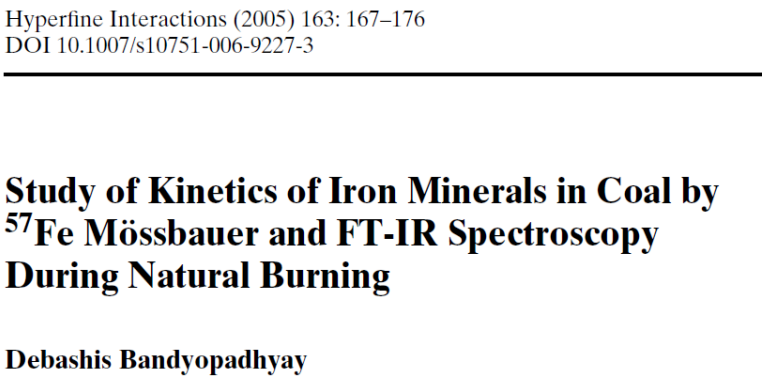
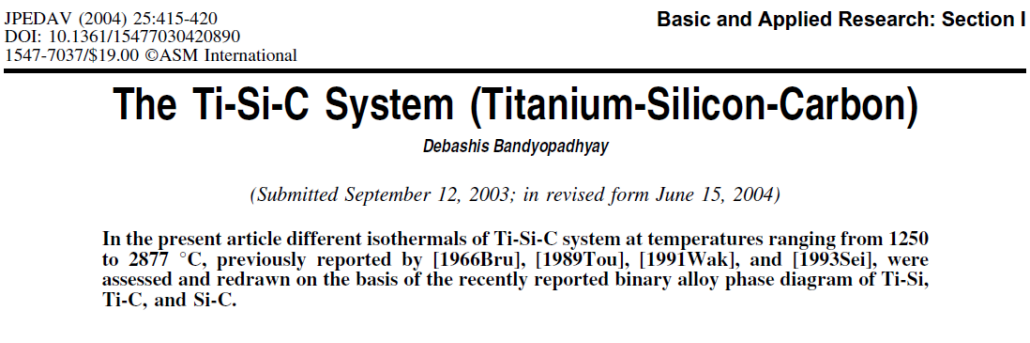
		
25	*Study of kinetics of iron minerals in coal by ^{57}Fe Mössbauer and FT-IR spectroscopy during natural burning,* ***Debashis Bandyopadhyay****, Hyperfine interactions 163 (1-4) (2005) 167-176, https://doi.org/10.1179/174328006X79490* 	***2005 IF 1.3***
24	*The Ti-Si-C system (titanium-silicon-carbon),* ***Debashis Bandyopadhyay****, Journal of phase equilibria and diffusion 25 (5), 415-420* 	***2004 IF 1.5***
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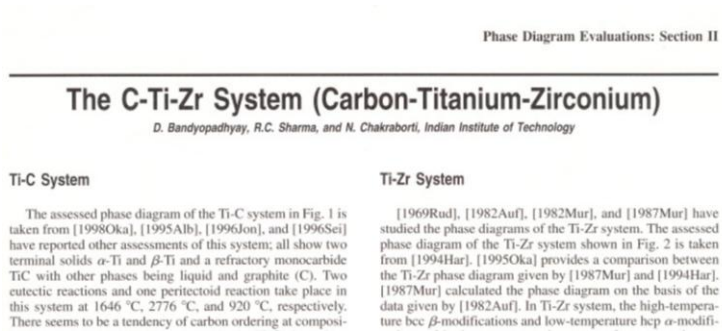
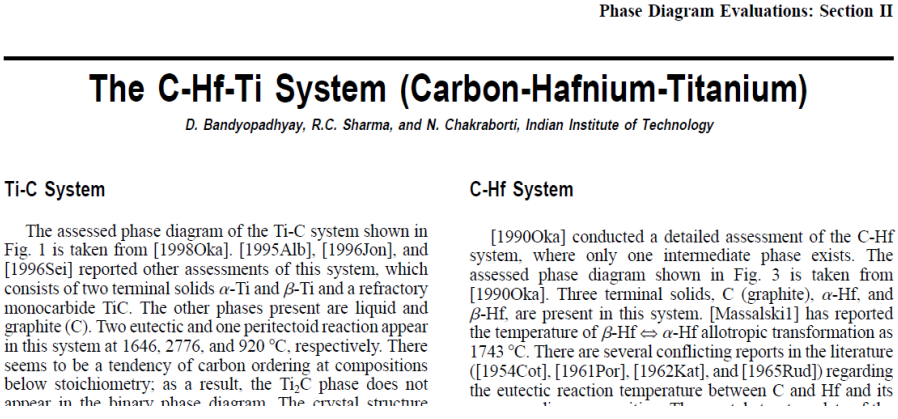
		
21	*Calculation of the Debye temperature and study of the lattice dynamics of $Fe_{80-x}Ni_xCr_{20}$ by ^{57}Fe Mössbauer spectroscopy,* ***D. Bandyopadhyay****, RM Singru, AK Majumdar, Zeitschrift für Metallkunde 92 (4), 367-369*	***2001***
20	*The C-Hf-Ti system (carbon-hafnium-titanium),* ***D. Bandyopadhyay****, RC Sharma, N Chakraborti Journal of phase equilibria 21 (6), 535-538* 	***2000*** ***IF*** ***1.5***
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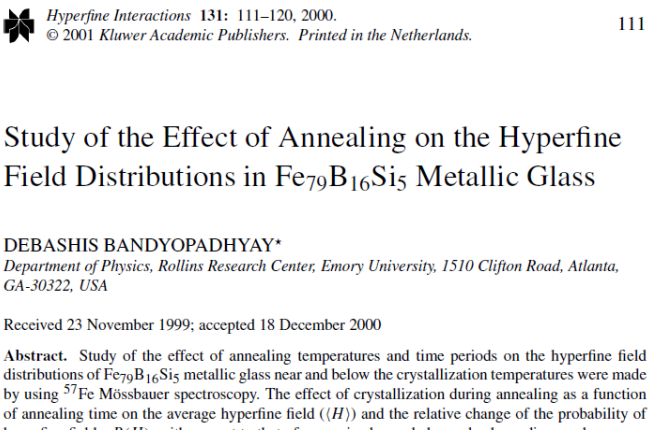
18	*Study of the effect of annealing on the hyperfine field distributions in Fe79B16Si5 Metallic Glass, D. Bandyopadhyay, Hyperfine Interactions, 131, 111-120* 	***2000*** ***IF*** ***1.3***
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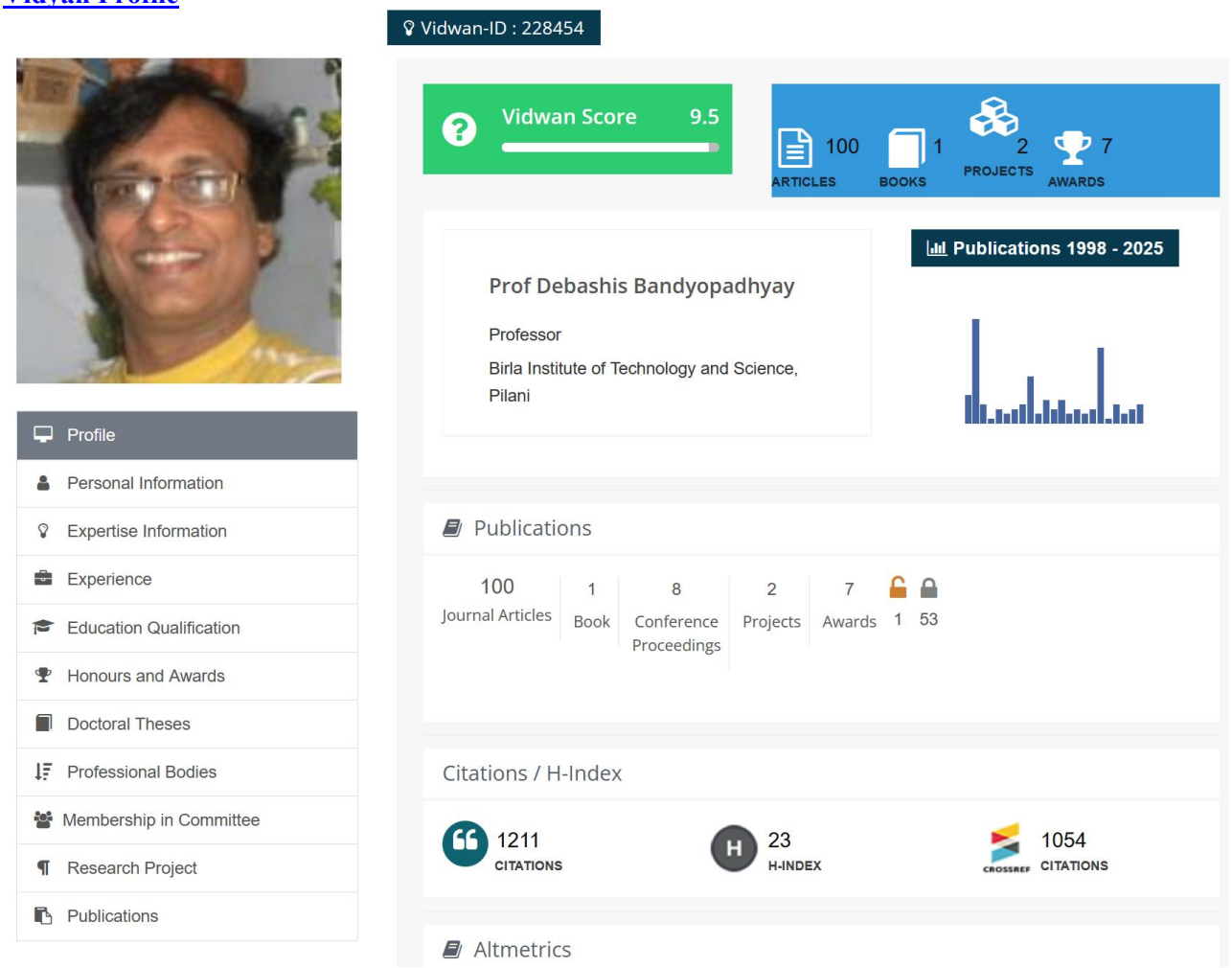
Vidyan Profile



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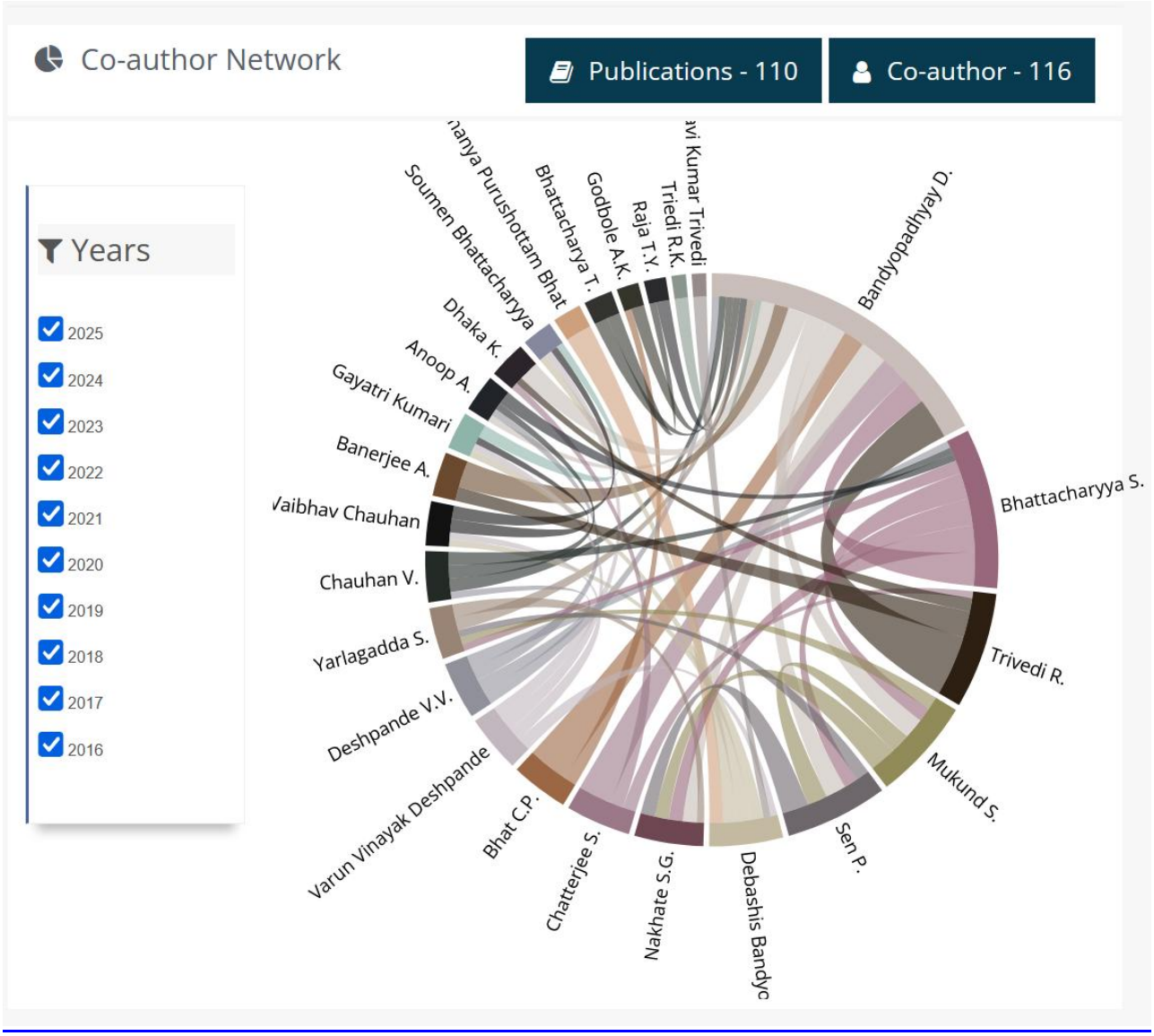
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