LIST OF PUBLICATIONS

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	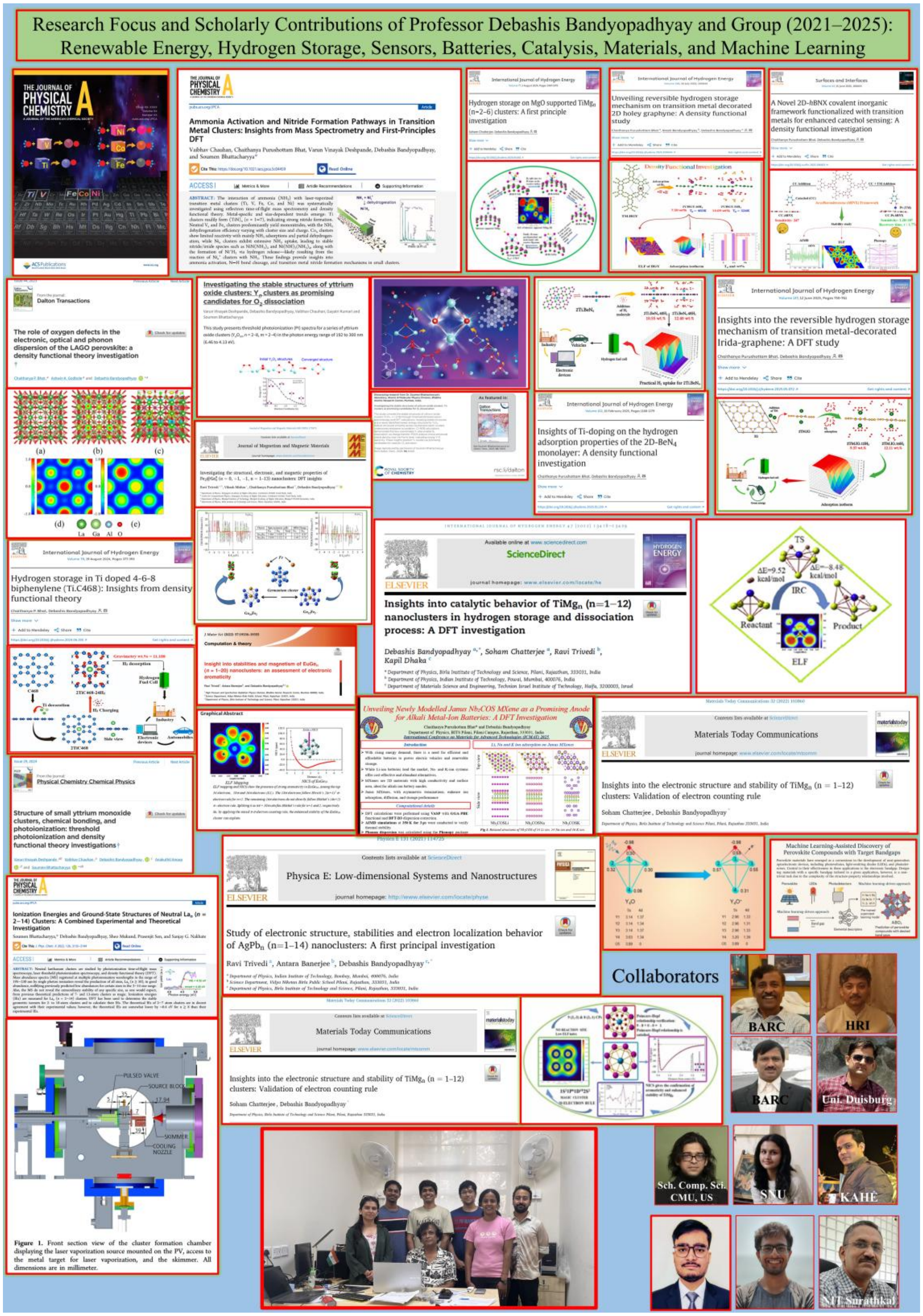	

Focus: Single authorship Invited review article with IF 16.8

Study of materials using Mössbauer spectroscopy, Debashis Bandyopadhyay, International materials reviews 51 (3) (2006) 171-208

2006 IF 16.8

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Journal
International Materials Reviews ›
Volume 51, 2006 - Issue 3

Study of materials using Mössbauer spectroscopy

D. Bandyopadhyay*

A comprehensive review is presented of the recent contributions Mössbauer spectroscopy has made in materials science and engineering. After a brief introduction to the basic methodology, examples of the application of ^{57}Fe and ^{119}Sn Mössbauer spectroscopy in both transmission and back-scattering mode are presented and discussed. Recent technological and software developments of this technique are also included. Coverage is further extended to recent, pertinent developments in space research and also in biological science and technology where Mössbauer techniques are very widely used. Efforts have also been made to cover applications to archaeological samples where Mössbauer spectroscopy is an important analytical tool.

Keywords: Archaeology, Biological science, Magnetic materials, Metallic glass, Minerals, Mössbauer spectroscopy, Nanomaterials, Space research, Steels

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2025 IF 2.8

THE JOURNAL OF PHYSICAL CHEMISTRY A
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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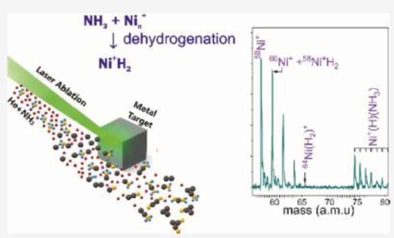
Ammonia Activation and Nitride Formation Pathways in Transition Metal Clusters: Insights from Mass Spectrometry and First-Principles DFT

Vaibhav Chauhan, Chaithanya Purushottam Bhat, Varun Vinayak Deshpande, Debashis Bandyopadhyay, and Soumen Bhattacharyya*

Cite This: https://doi.org/10.1021/acs.jpca.5c04459 Read Online

ABSTRACT: The interaction of ammonia (NH_3) with laser-vaporized transition metal clusters (Ti, V, Fe, Co, and Ni) was systematically investigated using reflectron time-of-flight mass spectrometry and density functional theory. Metal-specific and size-dependent trends emerge: Ti clusters readily form $(TiN)_n$ ($n = 1-7$), indicating strong nitride formation. Neutral V_n and Fe_n clusters predominantly yield mononitrides, with the NH_3 dehydrogenation efficiency varying with cluster size and charge. Co_n clusters show limited reactivity with mainly NH_3 adsorptions and partial dehydrogenation, while Ni_n clusters exhibit extensive NH_3 uptake, leading to stable nitride/imide species such as $NiN(NH_3)_4$ and $Ni(NH)_2(NH_3)_4$, along with the formation of Ni^+H_2 via hydrogen release—likely resulting from the reaction of Ni_n^+ clusters with NH_3. These findings provide insights into ammonia activation, N−H bond cleavage, and transition metal nitride formation mechanisms in small clusters.



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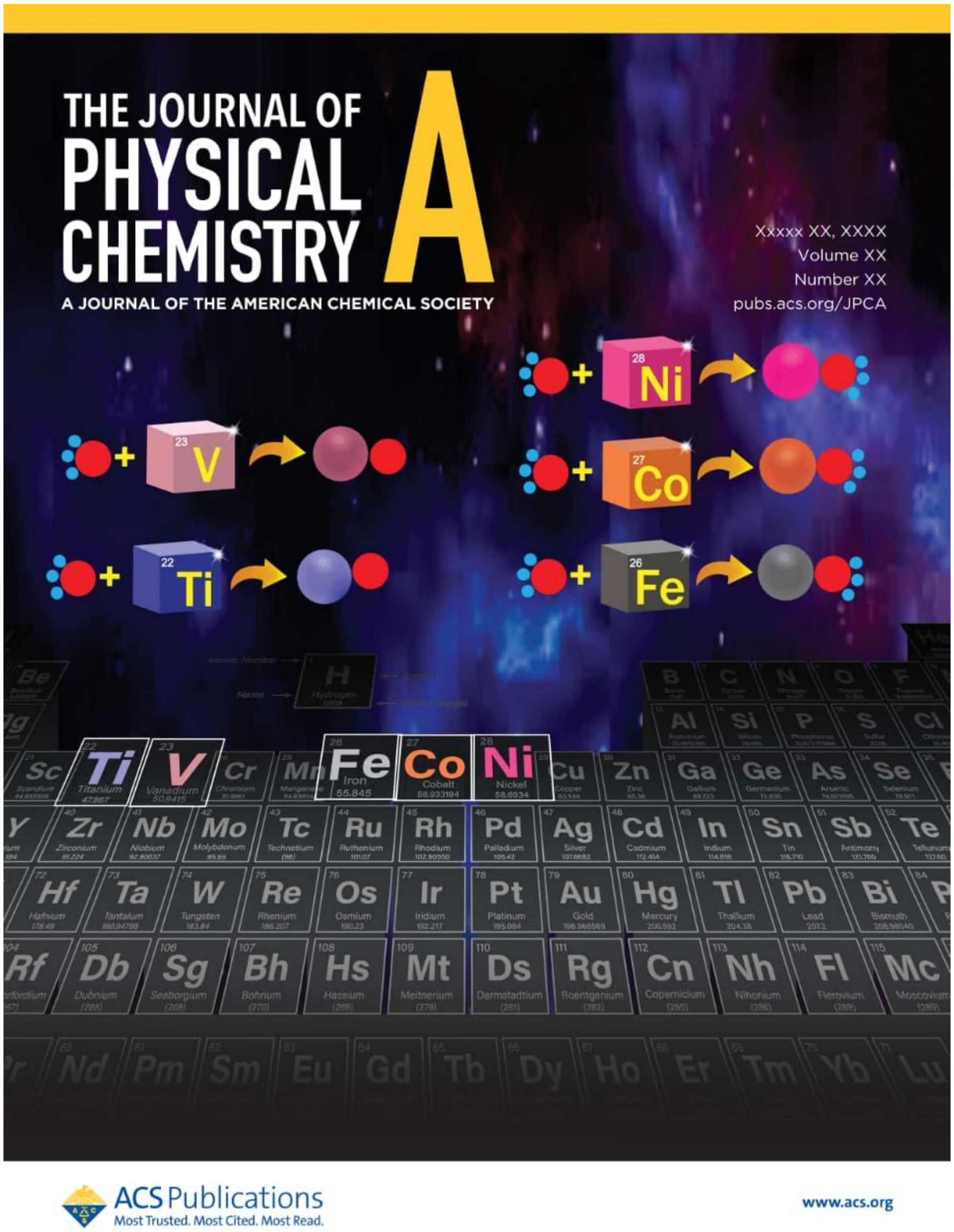

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Investigating the structural, electronic, and magnetic properties of $Fe_2@Ge_n^{\alpha}$ (α = 0, +1, −1, n = 1–13) nanoclusters: DFT insights

Ravi Trivedi [a,b], Vikash Mishra [c], Chaithanya Purushottam Bhat [d], Debashis Bandyopadhyay [d,*]

[a] Department of Physics, Karpagam Academy of Higher Education, Coimbatore 641021 Tamil Nadu, India
[b] Center for Computational Physics, Karpagam Academy of Higher Education, Coimbatore 641021 Tamil Nadu, India
[c] Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal 576104 Karnataka, India
[d] Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan 333031, India

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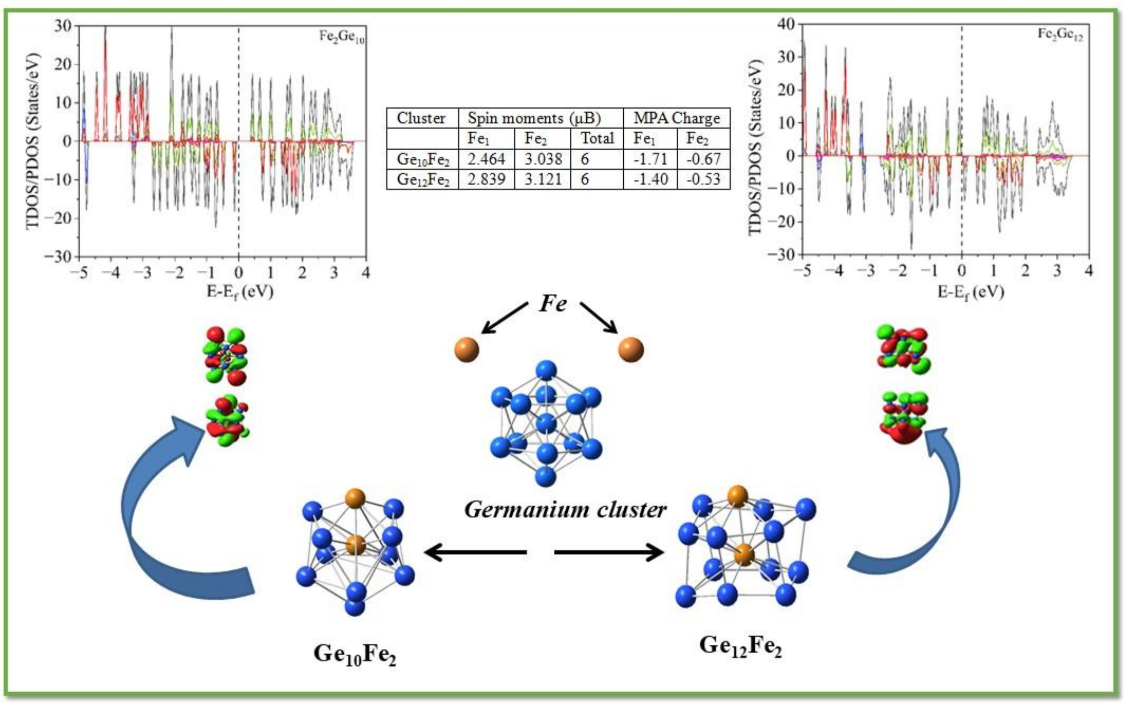

2005 IF 3.0

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*

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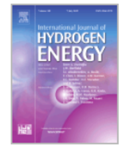

International Journal of Hydrogen Energy
Volume 148, 16 July 2025, 150044

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]

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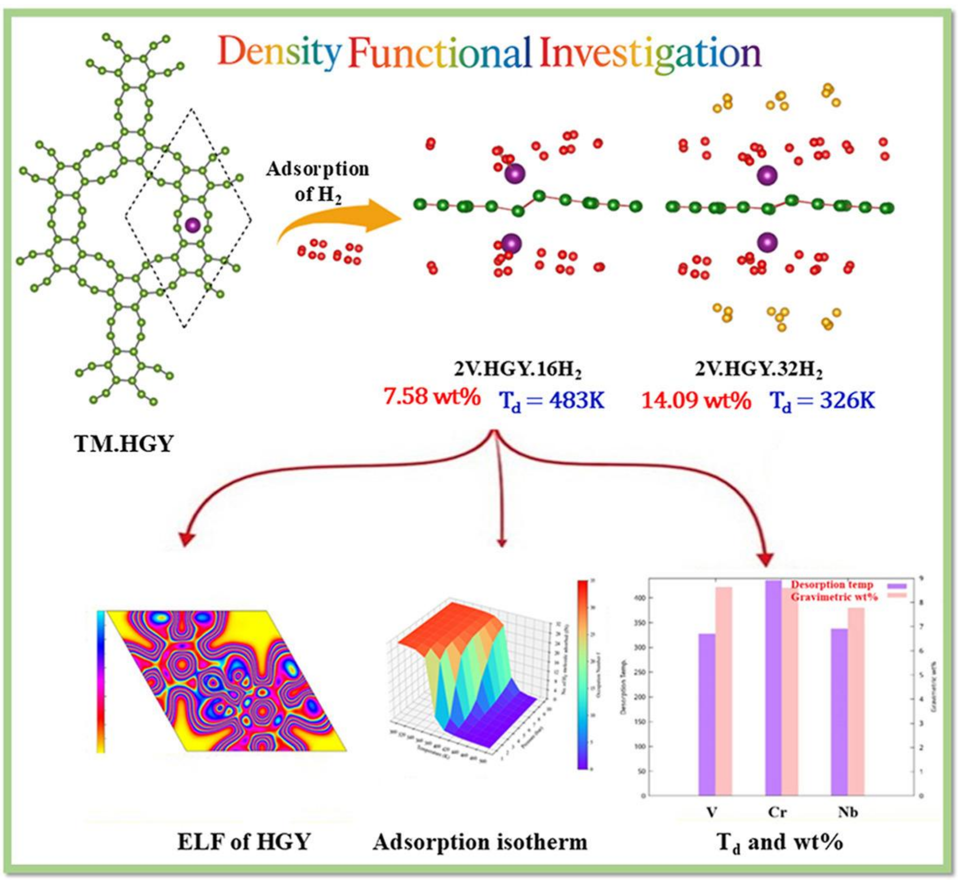

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<tr><td>63</td><td>Insights into the reversible hydrogen storage mechanism of transition metal-decorated Irida-graphene: A DFT study, Chithanya Purushottam Bhat, Debashis Bandyopadhyay, International Journal of Hydrogen Energy 137(2025) 750-761
https://doi.org/10.1016/j.ijhydene.2025.05.072

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

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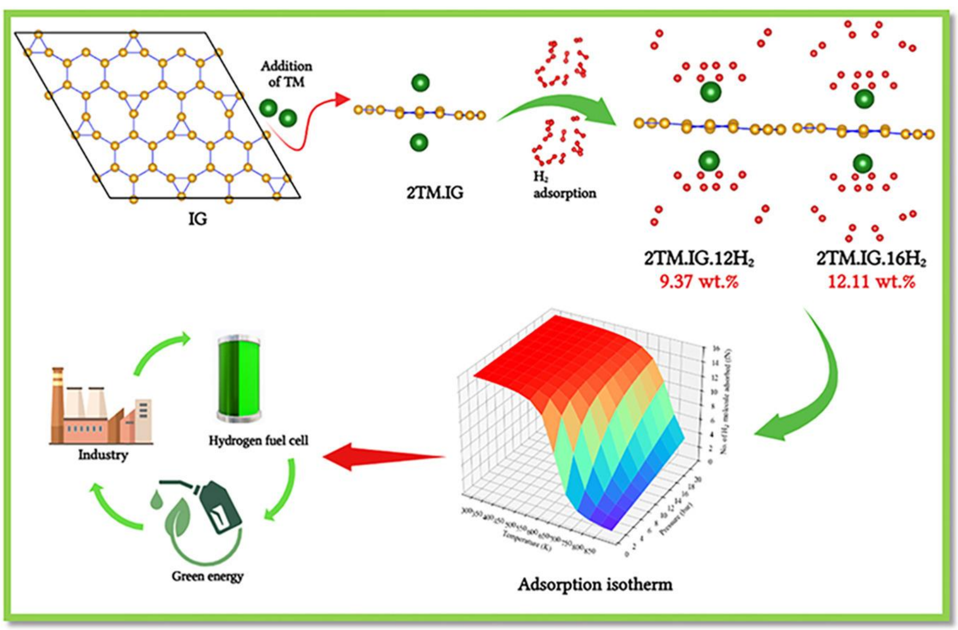
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<tr><td>62</td><td>A Novel 2D-hBNX Covalent Inorganic Framework Functionalized with Transition Metals for Enhanced Catechol Sensing: A Density Functional Investigation
Chaithanya Purushottam Bhat, Debashis Bandyopadhyay, Surfaces and Interfaces 67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

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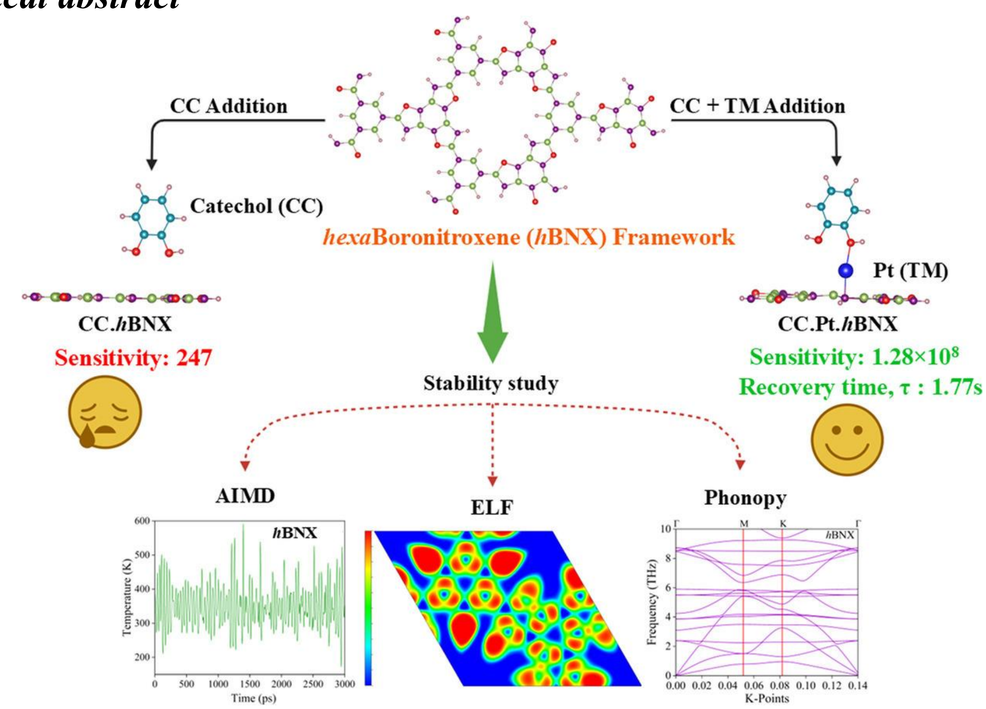
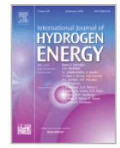


61	*Insights of Ti-doping on the hydrogen adsorption properties of the 2D-BeN4 monolayer: A density functional investigation, CP Bhat, D Bandyopadhyay* *International Journal of Hydrogen Energy 102 (2025) 1168-1179*	***2025 IF 8.3***

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



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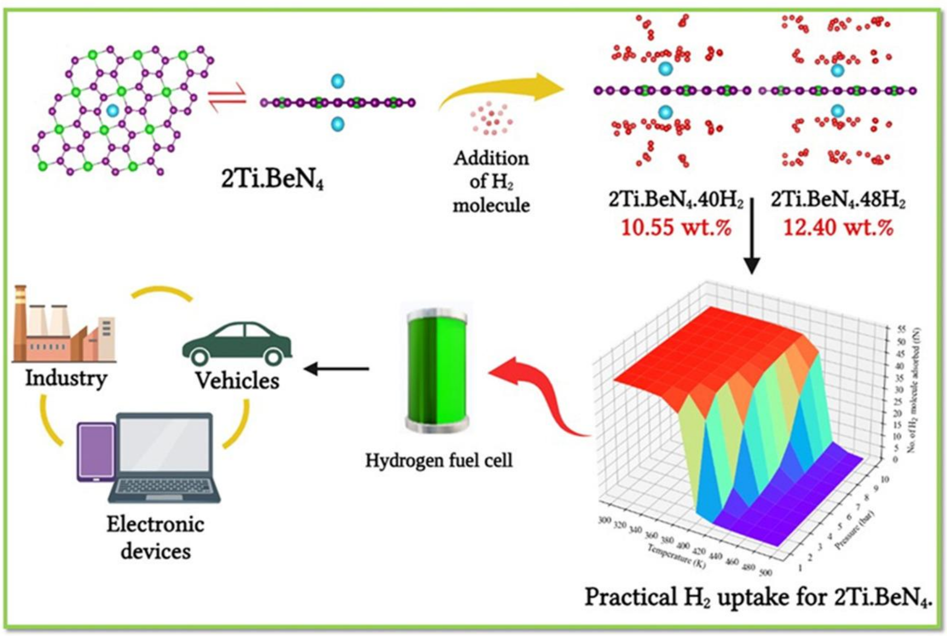

60	*Investigating the stable structures of yttrium oxide clusters: Y_n clusters as promising candidates for O_2 dissociation, Varun Vinayak Deshpande, Debashis Bandyopadhyay, Vaibhav Chauhan, Gayatri Kumari, Soumen Bhattacharyya, Dalton Transactions 54 (16), (2025) 6402-6410,*	***2025 IF 3.5***

Issue 16, 2025

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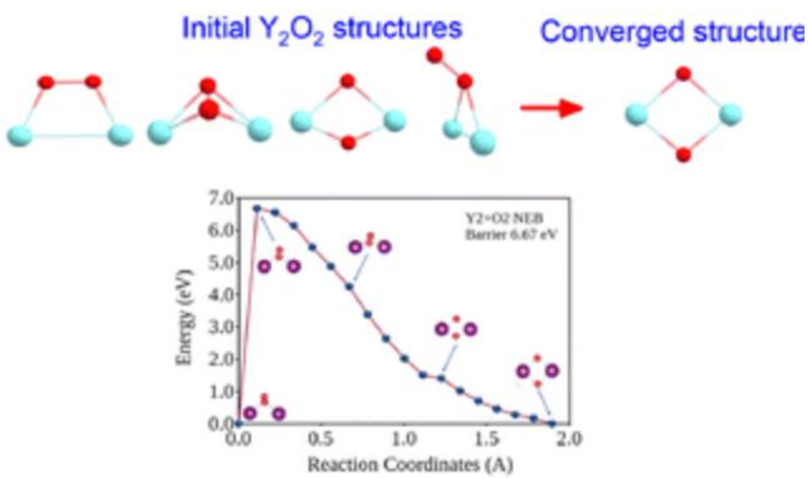
From the journal:
Dalton Transactions

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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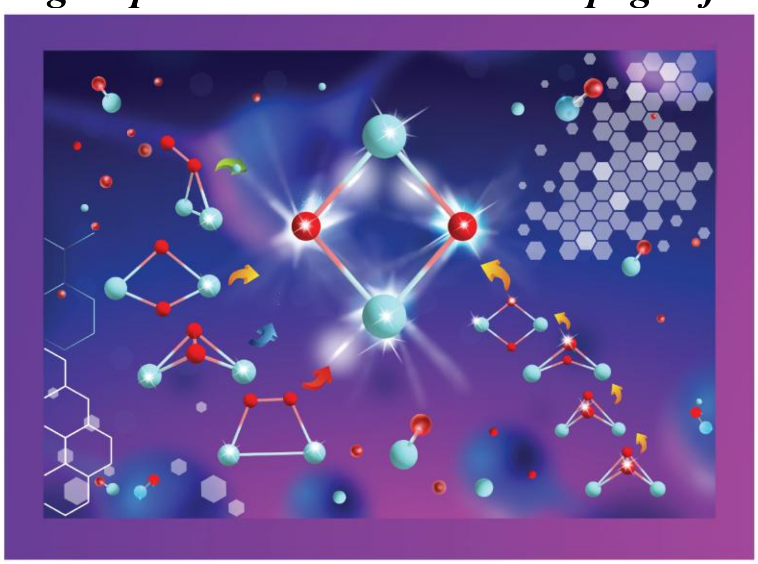

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<tr><td>59</td><td>Hydrogen storage in Ti doped 4-6-8 biphenylene (Ti. C468): Insights from density functional theory, Chaithanya Purushottam Bhat, Debashis Bandyopadhyay
International Journal of Hydrogen Energy 79 (2025) 377-393,
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Volume 79, 19 August 2024, Pages 377-393

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

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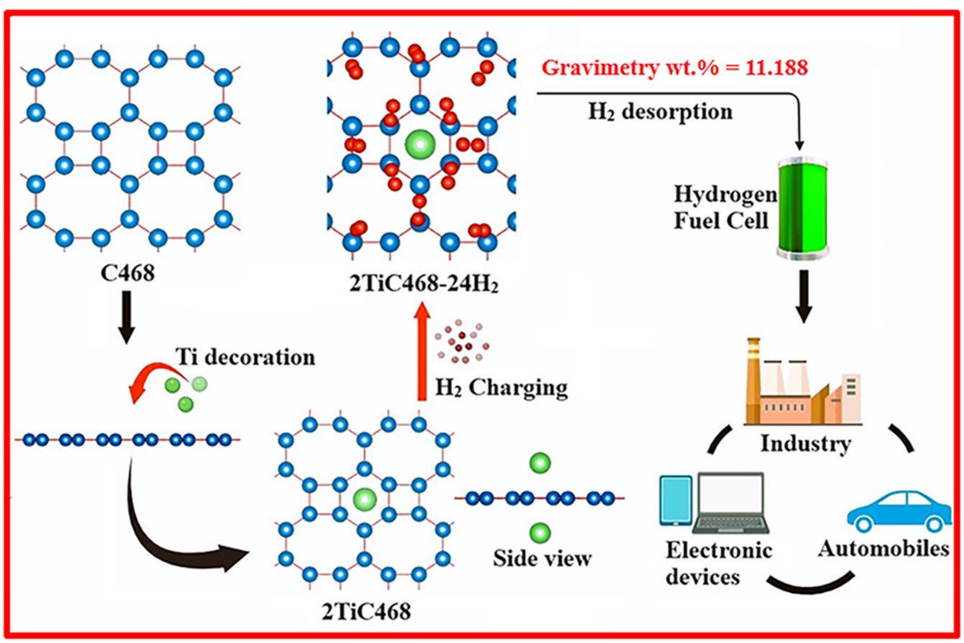
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<tr><td>58</td><td>Hydrogen storage on MgO supported TiMgn (n= 2–6) clusters: A first principle investigation, S Chatterjee, D Bandyopadhyay, International Journal of Hydrogen Energy 77, (2024) 1467-1475,</td><td>2024
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International 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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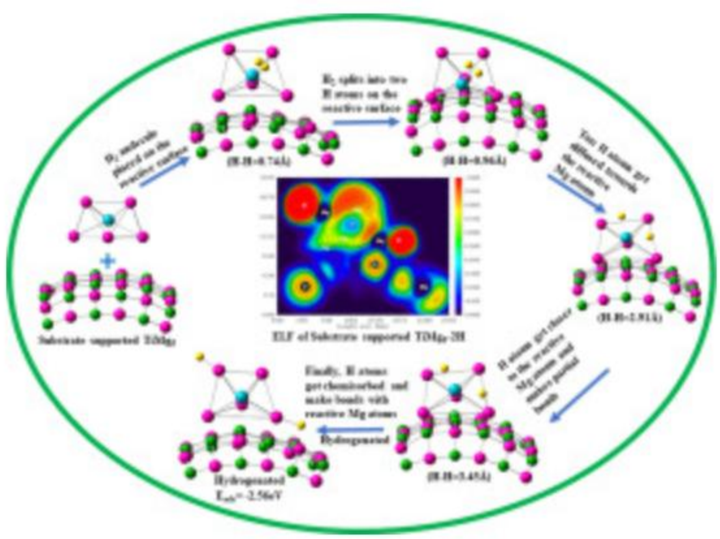

57	*Structure of small yttrium monoxide clusters, chemical bonding, and photoionization: threshold photoionization and density functional theory investigations, Varun Vinayak Deshpande, Vaibhav Chauhan, Debashis Bandyopadhyay, Anakuthil Anoop, Soumen Bhattacharyya,* ***Phys. Chem. Chem. Phys.****, 2024,****26****,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

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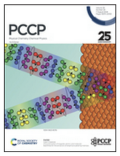
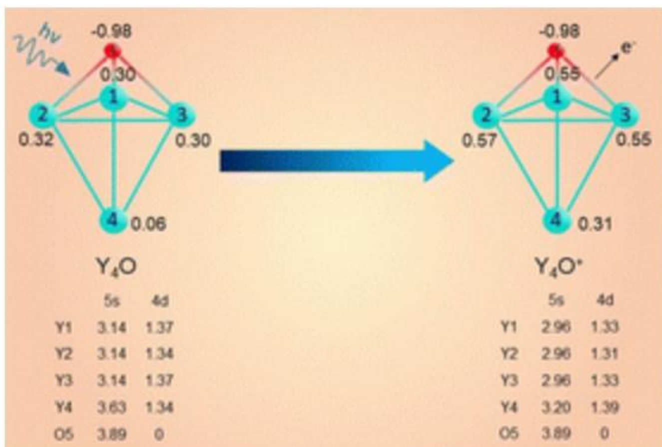


From the journal:
Physical Chemistry Chemical Physics

Structure of small yttrium monoxide clusters, chemical bonding, and photoionization: threshold photoionization and density functional theory investigations†

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***

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Dalton Transactions

The role of oxygen defects in the electronic, optical and phonon dispersion of the LAGO perovskite: a density functional theory investigation †
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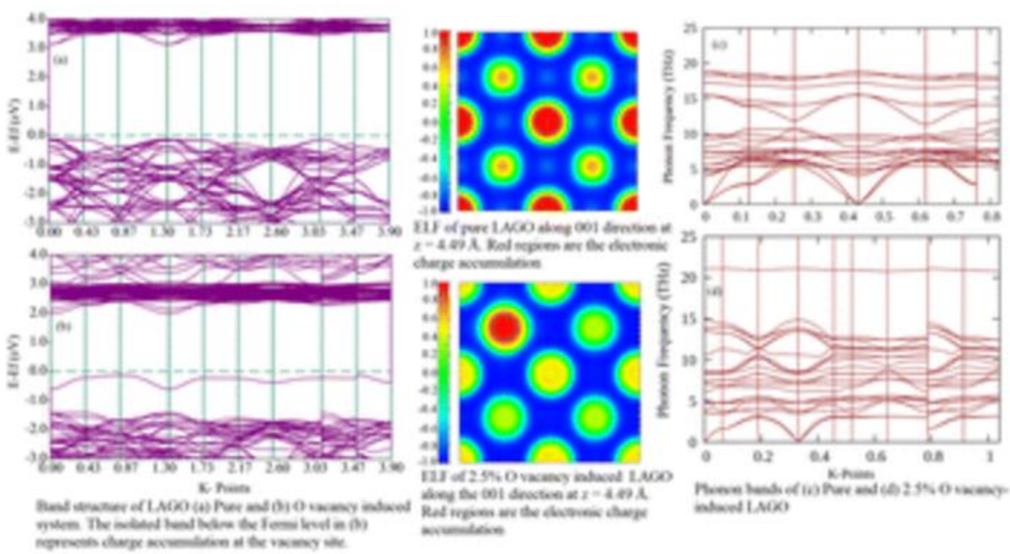
Chaithanya P. Bhat,[a] Ashwin K. Godbole[a] and Debashis Bandyopadhyay *[a]



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<td>55</td>
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<td>54</td>
<td>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</td>
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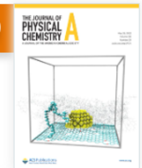
Ionization Energies and Ground-State Structures of Neutral La_n (n = 2–14) Clusters: A Combined Experimental and Theoretical Investigation

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

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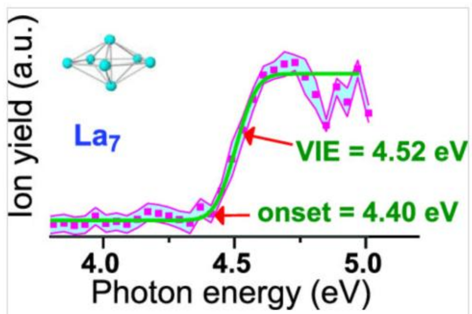
Abstract

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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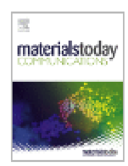
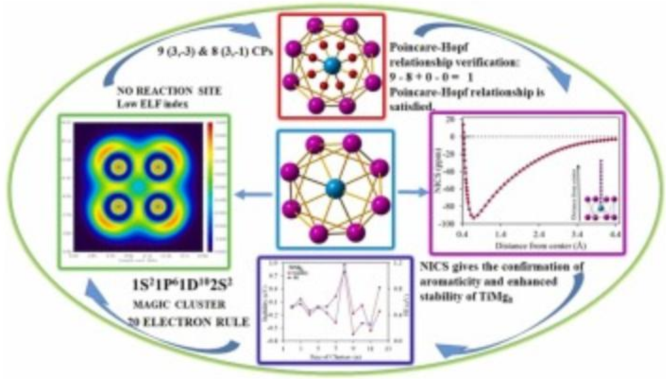


Volume 32, August 2022, 103860

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* *J Mater Sci* (2022) 57:19338–19355 **Computation & theory** Check for updates **Insight into stabilities and magnetism of $EuGe_n$ (n = 1–20) nanoclusters: an assessment of electronic aromaticity** Ravi Trivedi[1], Antara Banerjee[2], and Debashis Bandyopadhyay[3,*] [1] High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India [2] Science Department, Vidya Niketan Birla Public School, Pilani, Rajasthan 333031, India [3] Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan 333031, India	***2022 IF 3.5***

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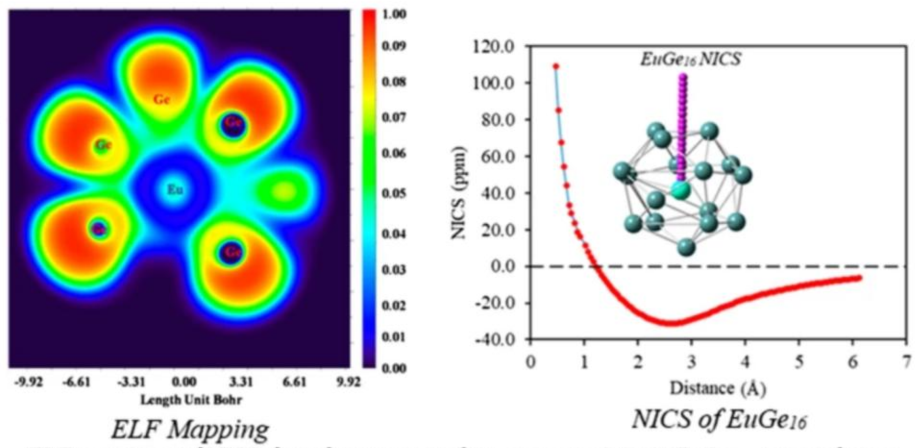

ELF Mapping *NICS of $EuGe_{16}$*

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 $6\pi + 10\pi$ 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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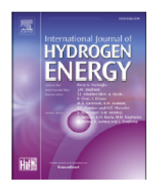
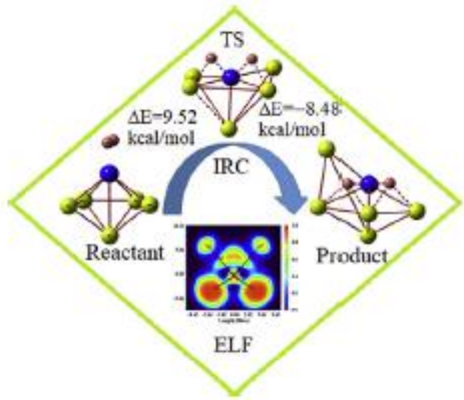


Insights into catalytic behavior of $TiMg_n$ (n=1–12) nanoclusters in hydrogen storage and dissociation process: A DFT investigation

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 Physica E 131 (2021) 114725 Contents lists available at ScienceDirect Physica E: Low-dimensional Systems and Nanostructures journal homepage: http://www.elsevier.com/locate/physe ELSEVIER 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	***2021 IF 2.9***
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* EPJ D Recognized by European Physical Society Atomic, Molecular, Optical and Plasma Physics 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	***2019 IF 1.5***

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

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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

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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.* **2016**

INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 41 (2016) 20113–20121

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International Journal of HYDROGEN ENERGY

CrossMark

Study of adsorption and dissociation pathway of H_2 molecule on Mg_nRh (n = 1–10) clusters: A first principle investigation

Ravi Trivedi, Debashis Bandyopadhyay*

Department of Physics, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, 333031, India

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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* **2016 IF 3.5**

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ROYAL SOCIETY OF CHEMISTRY

PAPER

Cite this: DOI: 10.1039/c6dt01252c

Magnetism, structures and stabilities of cluster assembled TM@Si nanotubes (TM = Cr, Mn and Fe): a density functional study†

Kapil Dhaka and Debashis Bandyopadhyay*

Received 31st March 2016, Accepted 4th July 2016
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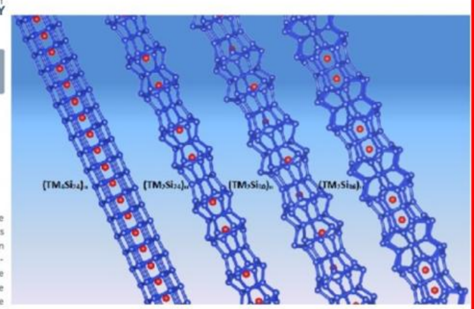
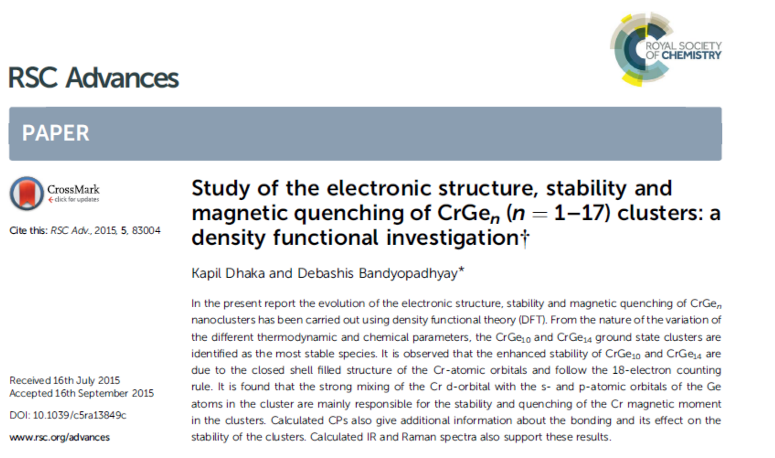
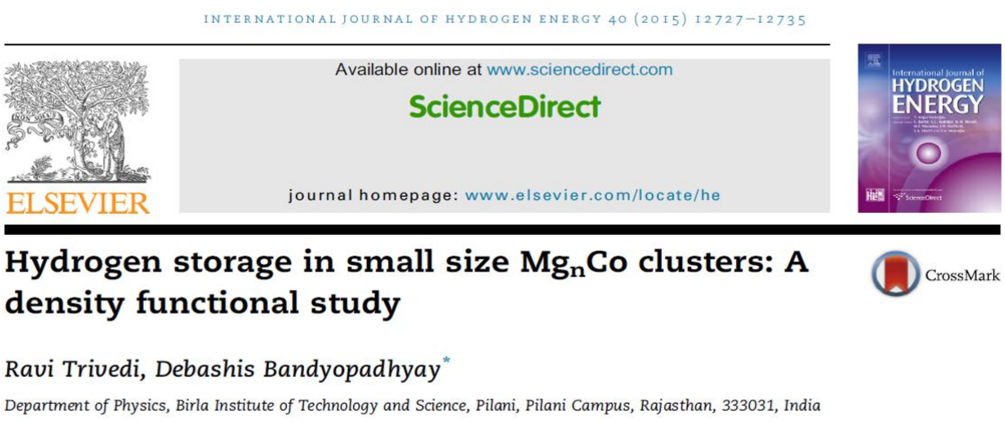
www.rsc.org/dalton

The present study reports transition metal (TM = Cr, Mn and Fe) doped silicon nanotubes with tunable band structures and magnetic properties by careful selection of cluster assemblies as building blocks using the first-principles density functional theory. We found that the transition metal doping and in addition, the hydrogen termination process can stabilize the pure silicon nanoclusters or cluster assemblies and then it could be extended as magnetic nanotubes with finite magnetic moments. Study of the band structures and density of states (DOS) of different empty and TM doped nanotubes (Type 1 to Type 4) show that these nanotubes are useful as metals, semiconductors, semi-metals and half-metals. These designer magnetic materials could be useful in spintronics and magnetic devices of nanoscale order.



Introduction

materials as building blocks is the prime focus of the nanotube research.[3–22] However, building of such materials has its

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 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 **Hydrogen storage in small size** Mg_nCo **clusters: A density functional study** Ravi Trivedi, Debashis Bandyopadhyay* Department of Physics, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, 333031, India	***2015 IF 8.3***
41	*Study of electronic properties, stabilities and magnetic quenching of molybdenum-doped germanium clusters: a density functional investigation, Ravi Trivedi, Kapil Dhaka,* ***Debashis Bandyopadhyay*** *RSC Advances 4 (2014) 64825-64834, https://doi.org/10.1039/C4RA11825A*	***2014 IF 4.6***

	RSC Advances ROYAL SOCIETY OF CHEMISTRY PAPER View Article Online View Journal | View Issue CrossMark Cite this: *RSC Adv.*, 2014, 4, 64825 **Study of electronic properties, stabilities and magnetic quenching of molybdenum-doped germanium clusters: a density functional investigation†** Ravi Trivedi, Kapil Dhaka and Debashis Bandyopadhyay* Evolution of electronic structures, properties and stabilities of neutral and cationic molybdenum encapsulated germanium clusters ($Mo@Ge_n$, n = 1 to 20) has been investigated using the linear combination of atomic orbital density functional theory method with effective core potential. From the variation of different thermodynamic and chemical parameters of the ground state clusters during the growth process, the stability and electronic structures of the clusters is explained. From the study of the distance-dependent nucleus-independent chemical shifts (NICS), we found that $Mo@Ge_{12}$ with hexagonal prism-like structure is the most stable isomer and possesses strong aromatic character. Density of states (DOS) plots of different clusters is then discussed to explain the role of d-orbitals of the Mo atom in hybridization. Quenching of the magnetic moment of the Mo atom with increase in the size of the cluster is also discussed. Finally, the validity of the 18-electron counting rule is applied to further explain the stability of the metallo-inorganic magic cluster $Mo@Ge_{12}$ and the possibility of Mo-based cluster-assembled materials is discussed. Received 5th October 2014 Accepted 3rd November 2014 DOI: 10.1039/c4ra11825a www.rsc.org/advances	
40	*Magnetic behavior in $Cr_2@Ge_n$ (1≤ n≤ 12) clusters: A density functional investigation, Kapil Dhaka, Ravi Trivedi, **Debashis Bandyopadhyay**, AIP Conference Proceedings, doi: 10.1063/1.4873009 1498, 1591* AIP | Proceedings **Magnetic behavior in Cr 2 @ Ge n (1n12) clusters: A density functional investigation** Kapil Dhaka, Ravi Trivedi, and Debashis Bandyopadhyay Citation: AIP Conference Proceedings **1591**, 1498 (2014); doi: 10.1063/1.4873009 View online: http://dx.doi.org/10.1063/1.4873009 View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1591?ver=pdfcov Published by the AIP Publishing	***2014***
39	*Shell Magnetism of Chromium Doped Germanium Superatom, Kapil Dhaka, **Debashis Bandyopadhyay**, Advanced Science Letters 20 (3), 1135-1137*	***2014***
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@Ge_n (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*](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***
34	*New Insights into Applicability of Electron-Counting Rules in Transition Metal Encapsulating Ge Cage Clusters,* ***Debashis Bandyopadhyay****, Prabshran Kaur, Prasenjit Sen, The Journal of Physical Chemistry A 114 (50) (2010) 12986-12991,* [*https://doi.org/10.1021/jp106354d*](https://doi.org/10.1021/jp106354d)	***2010 IF 2.7***

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<tr><td></td><td>12986 J. Phys. Chem. A 2010, 114, 12986–12991

New Insights into Applicability of Electron-Counting Rules in Transition Metal Encapsulating Ge Cage Clusters

Debashis Bandyopadhyay,[†] Prabhsharan Kaur,[‡] and Prasenjit Sen*,[§]
Physics Group, Birla Institute of Technology and Science, Pilani, Rajasthan, India, Physics Department, National Institute of Technology, Hamirpur, HP, India, and Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Allahabad 211019, India
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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</td><td></td></tr>
<tr><td>33</td><td>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, Prasenjit Sen, The Journal of Physical Chemistry A 114 (4) (2010) 1835-1842, https://doi.org/10.1021/jp905561n

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*,[‡]
Physics Group, Birla Institute of Technology and Science, Pilani - 333031, Rajasthan, India, and Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Allahabad-211019, U.P, India
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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.</td><td>2010
IF
2.7</td></tr>
<tr><td>32</td><td>Effect of Transition Metal Doping on Hydrogenated Germanium Nanocages: A Density Functional Investigation, M Kumar, BJ Singh, S Kajjam, D. Bandyopadhyay
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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]
[1]Physics Group, [2]Electronics and Instrumentation Group, Birla Institute of Technology and Science, Pilani, Rajasthan 333031, India

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</td><td>2010</td></tr>
<tr><td>31</td><td>Density functional study of the electronic structure and properties of lithium intercalated graphite, Debashis Bandyopadhyay, The European Physical Journal D 54 (3), 643-655,
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Eur. Phys. J. D **54**, 643–655 (2009)
DOI: 10.1140/epjd/e2009-00189-2

THE EUROPEAN PHYSICAL JOURNAL D

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

D. Bandyopadhyay[a]

Physics Group, Birla Institute of Technology and Sciences, Pilani, 333031 Rajasthan, India

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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

30 *Study of pure and doped hydrogenated germanium cages: a density functional investigation, Debashis Bandyopadhyay, Nanotechnology 20 (27), 275202,* http://doi.org/10.1088/0957-4484/20/27/275202 — ***2009 IF 2.9***

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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

Debashis Bandyopadhyay

Physics Group, Birla Institute of Technology and Science, Pilani, Rajasthan-333031, India

E-mail: Debashis.bandy@gmail.com, rajuban@gmail.com and bandy@bits-pilani.ac.in

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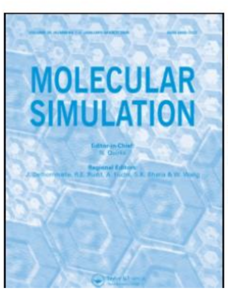
Abstract
In this paper we present an *ab initio* electronic-structure calculation performed using density functional theory (DFT) with a polarized basis set (SDD) within the spin polarized generalized gradient approximation for pure and divalent transition metal doped hydrogenated germanium nanocluster 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

29 *The study of the electronic structures and properties of pure and transition metal-doped silicon nanoclusters: a density functional theory approach,* ***Debashis Bandyopadhyay****, Molecular Simulation 35 (5), 381-394,* https://doi.org/10.1080/08927020802603598 — ***2009***



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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

Debashis Bandyopadhyay [a]
[a] Department of Physics, Birla Institute of Technology and Science, Pilani, India

First Published:April2009

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*](https://doi.org/10.1016/j.chemphys.2008.08.017)	***2008 IF 3.8***

Chemical Physics 353 (2008) 170–176

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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

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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.

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*](https://doi.org/10.1063/1.3000657)	***2008 IF 2.7***

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]

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	Taylor & Francis Online Journal International Materials Reviews › Volume 51, 2006 - Issue 3 **Study of materials using Mössbauer spectroscopy** **D. Bandyopadhyay*** A comprehensive review is presented of the recent contributions Mössbauer spectroscopy has made in materials science and engineering. After a brief introduction to the basic methodology, examples of the application of ^{57}Fe and ^{119}Sn Mössbauer spectroscopy in both transmission and back-scattering mode are presented and discussed. Recent technological and software developments of this technique are also included. Coverage is further extended to recent, pertinent developments in space research and also in biological science and technology where Mössbauer techniques are very widely used. Efforts have also been made to cover applications to archaeological samples where Mössbauer spectroscopy is an important analytical tool. **Keywords:** Archaeology, Biological science, Magnetic materials, Metallic glass, Minerals, Mössbauer spectroscopy, Nanomaterials, Space research, Steels	
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*](https://doi.org/10.1179/174328006X79490) Hyperfine Interactions (2005) 163: 167–176 DOI 10.1007/s10751-006-9227-3 **Study of Kinetics of Iron Minerals in Coal by ^{57}Fe Mössbauer and FT-IR Spectroscopy During Natural Burning** **Debashis Bandyopadhyay**	***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* JPEDAV (2004) 25:415-420 DOI: 10.1361/15477030420890 1547-7037/$19.00 ©ASM International **Basic and Applied Research: Section I** **The Ti-Si-C System (Titanium-Silicon-Carbon)** *Debashis Bandyopadhyay* *(Submitted September 12, 2003; in revised form June 15, 2004)* **In the present article different isothermals of Ti-Si-C system at temperatures ranging from 1250 to 2877 °C, previously reported by [1966Bru], [1989Tou], [1991Wak], and [1993Sei], were assessed and redrawn on the basis of the recently reported binary alloy phase diagram of Ti-Si, Ti-C, and Si-C.**	***2004 IF 1.5***
23	*Study of hyperfine field distributions and local magnetic order of $Fe_{80-x}Ni_xCr_{20}$ alloys by ^{57}Fe Mossbauer spectroscopy,* ***Debashis Bandyopadhyay****, ICAMMP-2002: International Conference on Advances in Materials Processing ...*	***2002***
22	*The C-Ti-Zr System (Carbon–Zirconium-Titanium),* ***D. Bandyopadhyay****, RC Sharma, N Chakraborti J. Phase Equilibria and Diffusion 22 (1), 61*	***2001 IF 1.5***

	Phase Diagram Evaluations: Section II **The C-Ti-Zr System (Carbon-Titanium-Zirconium)** *D. Bandyopadhyay, R.C. Sharma, and N. Chakraborti, Indian Institute of Technology* **Ti-C System** The assessed phase diagram of the Ti-C system in Fig. 1 is taken from [1998Oka], [1995Alb], [1996Jon], and [1996Sei] have reported other assessments of this system; all show two terminal solids α-Ti and β-Ti and a refractory monocarbide TiC with other phases being liquid and graphite (C). Two eutectic reactions and one peritectoid reaction take place in this system at 1646 °C, 2776 °C, and 920 °C, respectively. There seems to be a tendency of carbon ordering at composi- **Ti-Zr System** [1969Rud], [1982Auf], [1982Mur], and [1987Mur] have studied the phase diagrams of the Ti-Zr system. The assessed phase diagram of the Ti-Zr system shown in Fig. 2 is taken from [1994Har]. [1995Oka] provides a comparison between the Ti-Zr phase diagram given by [1987Mur] and [1994Har]. [1987Mur] calculated the phase diagram on the basis of the data given by [1982Auf]. In Ti-Zr system, the high-temperature bcc β-modifications and low-temperature hcp α-modifi-	
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* Phase Diagram Evaluations: Section II **The C-Hf-Ti System (Carbon-Hafnium-Titanium)** *D. Bandyopadhyay, R.C. Sharma, and N. Chakraborti, Indian Institute of Technology* **Ti-C System** The assessed phase diagram of the Ti-C system shown in Fig. 1 is taken from [1998Oka]. [1995Alb], [1996Jon], and [1996Sei] reported other assessments of this system, which consists of two terminal solids α-Ti and β-Ti and a refractory monocarbide TiC. The other phases present are liquid and graphite (C). Two eutectic and one peritectoid reaction appear in this system at 1646, 2776, and 920 °C, respectively. There seems to be a tendency of carbon ordering at compositions below stoichiometry; as a result, the Ti_2C phase does not **C-Hf System** [1990Oka] conducted a detailed assessment of the C-Hf system, where only one intermediate phase exists. The assessed phase diagram shown in Fig. 3 is taken from [1990Oka]. Three terminal solids, C (graphite), α-Hf, and β-Hf, are present in this system. [Massalski1] has reported the temperature of β-Hf $\Leftrightarrow$ α-Hf allotropic transformation as 1743 °C. There are several conflicting reports in the literature ([1954Cot], [1961Por], [1962Kat], and [1965Rud]) regarding the eutectic reaction temperature between C and Hf and its	***2000 IF 1.5***
19	*Study of the roasting of chalcopyrite minerals by ^{57}Fe Mössbauer spectroscopy, D. Bandyopadhyay, RM Singru, AK Biswas, Minerals engineering 13 (8), 973-978*	***2000***
18	*Study of the effect of annealing on the hyperfine field distributions in Fe79B16Si5 Metallic Glass, D. Bandyopadhyay, Hyperfine Interactions, 131, 111-120* *Hyperfine Interactions* **131:** 111–120, 2000. 111 © 2001 *Kluwer Academic Publishers. Printed in the Netherlands.* Study of the Effect of Annealing on the Hyperfine Field Distributions in $Fe_{79}B_{16}Si_5$ Metallic Glass DEBASHIS BANDYOPADHYAY* *Department of Physics, Rollins Research Center, Emory University, 1510 Clifton Road, Atlanta, GA-30322, USA* Received 23 November 1999; accepted 18 December 2000 **Abstract.** Study of the effect of annealing temperatures and time periods on the hyperfine field distributions of $Fe_{79}B_{16}Si_5$ metallic glass near and below the crystallization temperatures were made by using ^{57}Fe Mössbauer spectroscopy. The effect of crystallization during annealing as a function of annealing time on the average hyperfine field ($\langle H \rangle$) and the relative change of the probability of	***2000 IF 1.3***
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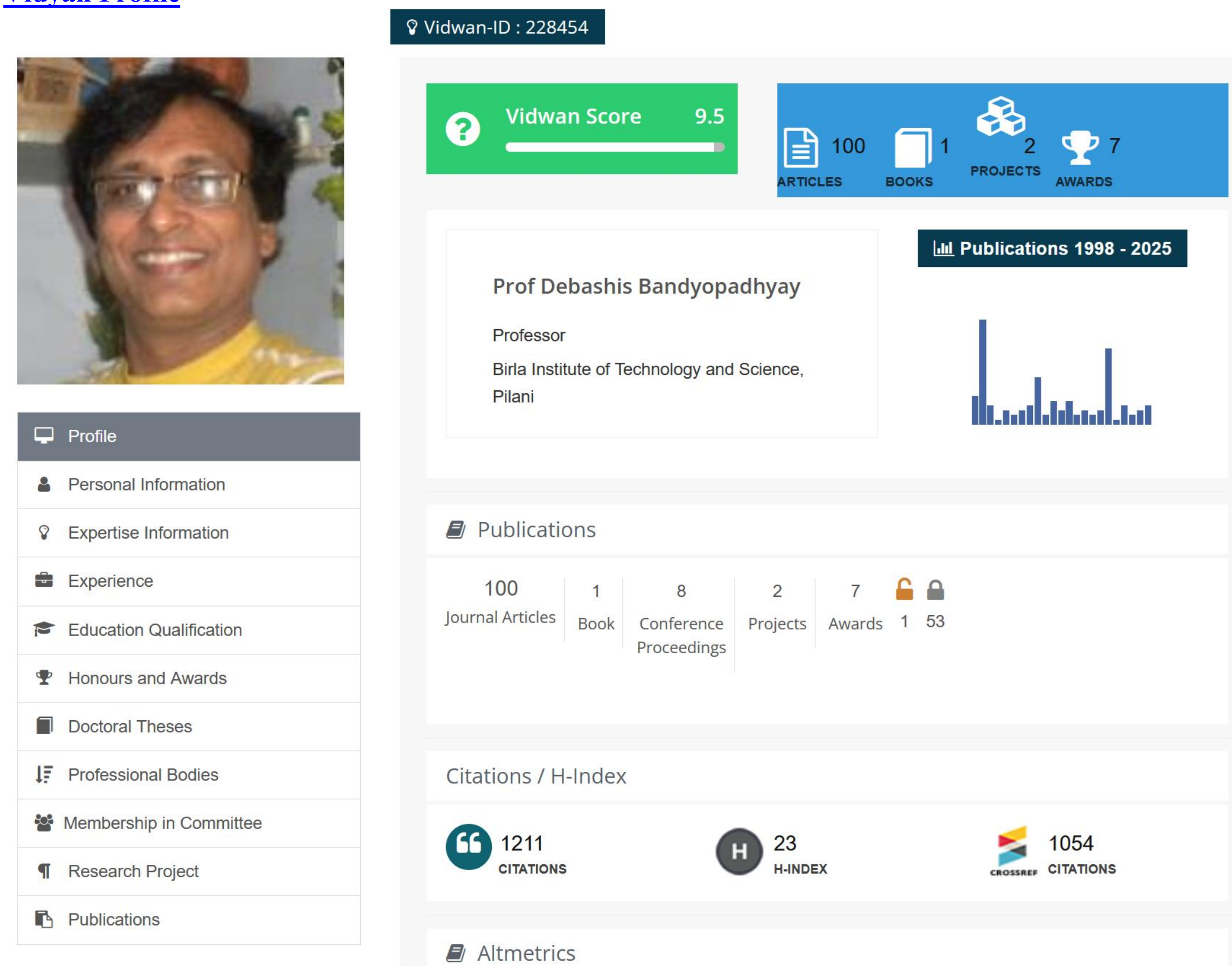
[Vidyan Profile]



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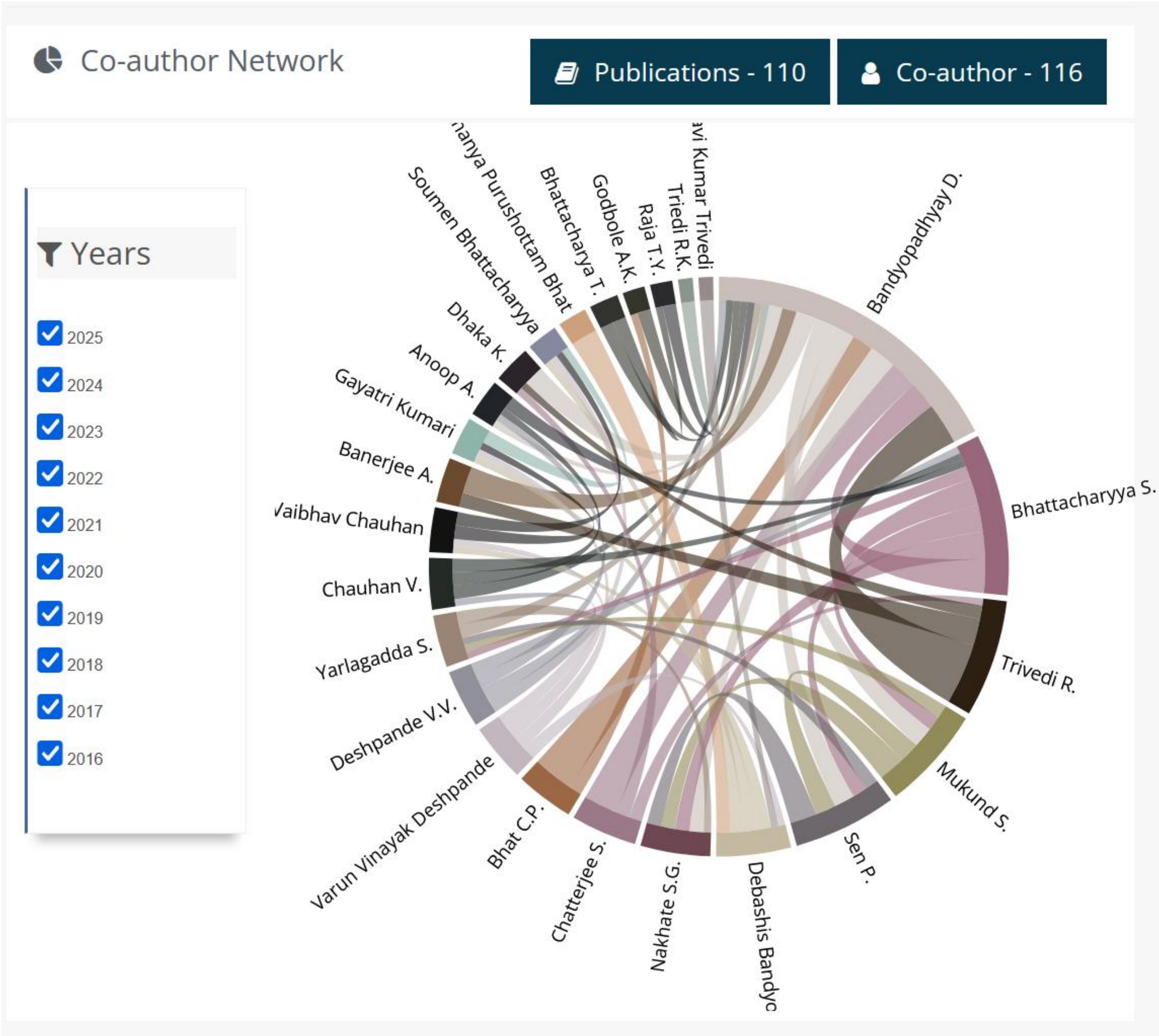
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Debashis Bandyopadhyay

Professor, Department of Physics, BITS, Pilani
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