Application for Assistant Professor Chemistry

Chhatrapati Shivaji Maharaj University

Panvel, Navi Mumbai, Maharashtra, 410206

Respected Madam/Sir,

I would like to be considered for the position of Assistant Professor Chemistry as advertised. I have the necessary skills and qualifications for this post, as well as the necessary experience.

I received a B.Sc. in Chemistry from Vidyasagar University, a M.Sc. in Chemistry from Pt. Ravishankar Shukla University, and a Ph.D. (Thesis Title :- Electronic structure of nano clusters and cluster molecule interactions) in Chemistry from Visva Bharati University under Prof. Pranab Sarkar (Visva-Bharati University) and Prof. Chiranjib Majumdar (Bhabha Atomic Research Centre), in 2015. Subsequently I have moved to University of Seoul and Pohang University of Science and Technology, South Korea for post-doctoral experience under Prof. Jeong Woo Han (Editor - Molecular Catalysis). I also worked as a visiting researcher at KTH Royal Institute of Technology, Stockholm with Prof. Tore Brinck. Presently I am working as guest faculty at Hemvati Nandan Bahuguna Garhwal University (A Central University), Uttarakhand.

I work on Computational Materials Chemistry. More specifically, I use Quantum Chemistry through various software for predicting and complementing chemical phenomena. My computational research has led to synthesis of single atom catalysts for electrochemical production of hydrogen and hydrogen peroxide (ACS Energy Lett. 4, 2019, 126-132, Adv. Energy Mater. 8, 2018, 1701476). This research also helped to understand the role of the catalyst for methane conversion to valuable chemicals (ChemSusChem 2020, 13, 1–6). During my PhD I performed electronic structure calculations of metal clusters and surfaces and their interaction with molecules. Presently I am trying to find a suitable catalyst for the nitrogen reduction reaction through an environment friendly way to bypassing the Haber Bosh process of current industrial ammonia production having environmental impact.

I am highly interested in join in your institution. I therefore sincerely request you for this position. Please find attached application and all supporting documents for your kind consideration. I look forward to hearing from you regarding next steps.

Yours sincerely,

Suman Kalyan Sahoo

Google Scholar

https://scholar.google.co.in/citations?user=yrDxXVcAAAAJ&hl=en

Curriculum Vitae

Suman Kalyan Sahoo

Date of birth: 7th August 1982

Nationality: Indian

Marital status: Married

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Educational Qualifications:

- Ph. D. (Chemistry), Visva-Bharati, West-Bengal, India (January,2009 - May,2015)
  Title of the Thesis: "***Electronic structure of nanoclusters and cluster-molecule interactions"***
- M.Sc. (Physical Chemistry), Pt. Ravishankar Shukla University, Chhattisgarh, India (April, 2004 – July,2006)
- B.Sc. (Chemistry), Vidyasagar University, West-Bengal, India (April,2000 – April,2003)

Scolarastic Achievements:

- Awarded Senior Research Fellowship sponsored by Council of Scientific and Industrial Research (CSIR), India, 2012.
- Awarded Junior Research Fellowship sponsored by Board of Research in Nuclear Sciences (BRNS), India, 2009.
- Worked as university research fellow in Kalyani University in a project " Synthesis of polymer anchored metal complex catalyst and their catalytic applications" (September,2007 - November, 2008)
- Worked as a Lecturer in Ramnagar College, Vidyasagar University (August,2006 – August,2007).
- Qualified joint CSIR-UGC National Eligibility Test (NET)-Dec 2006, Chemical Sciences.
- All India 461th rank in Graduate Aptitude Test for Engineers (GATE)-2007, Chemistry.

Postdoctoral Experience:

- **(2019-2021)**

  Visiting Researcher

  KTH Royal Institute of Technology, 100 44 Stockholm, Sweden
- (**2018 – 2019**)
  Postdoctoral Research Associate, Pohang University of Science and Technology (POSTECH), South Korea.
- (**2016 – 2018**)
  Postdoctoral Research Associate, University of Seoul, South Korea.
- **(2015 – 2016)**
  Postdoctoral Research Associate, Visva-Bharati, West-Bengal, India.

Membership of Professional societies:

Life member, Society of Material Chemistry, Mumbai, India.

My Research activities:

Using computational methods such as state-of-the-art Density Functional Theory (DFT) calculations, the major focus of my research efforts is on the modelling of materials with desired properties for a wide range of important applications as described below.

Electrochemical N_2 reduction reaction to ammonia production.

Hydrogen evolution and water dissociation

Hydrogen (H_2) is one of the most important raw material for petroleum refining, synthesizing ammonia-based fertilizers and environment-benign hydrogen fuel. The electrochemical hydrogen evolution reaction (HER) coupled to renewable energy sources is a potential sustainable source of H_2. Platinum is the most active HER catalyst, but cannot be used commercially for its high cost and scarcity. Finding a way to reduce the cost of HER catalyst is a solution to this problem.

- A search to boost the use of TiC as an alternative of conventional carbon material as electrocatalyst support is reported. In this regard, with the help of density functional theory, we explore the stability and activity of transition metal single atom (M= Cu, Ag, Au, Ni, Pd, Pt) on the TiC surface. We find the carbon vacancy, which is very common in experimental findings

helps to stabilize these single atom on this surface. HER activity of these catalyst has also been discussed and we find the Pt/TiC is a very good catalyst.

- We explore the structural and electronic properties of SnO_2 (110), TiO_2 (110) & $Ti_{0.5}Sn_{0.5}O_2$ (110) surfaces and then we study the energetics of molecular water adsorption on these surfaces. However, there is a significant difference in the adsorption behavior in terms of chemical bonding. While for TiO_2 (110) surface, water molecules are adsorbed without losing its molecular identity, on the SnO_2 (110) surface water molecules prefer dissociative adsorption. We also performing some calculation on gold clusters deposited on this surface.

H_2O_2 Synthesis

Presently, H_2O_2 is produced by the anthraquinone process, which is an energy demanding multi-electron process and require large plants. However, small-scale onsite production of hydrogen peroxide in remote areas is a challenge. Electrochemical synthesis of hydrogen peroxide (H_2O_2) in fuel cell is an attractive alternative to this anthraquinone process, which also generate electricity. Nevertheless, the major challenge in this field to finds a suitable material that selectively reduced O_2 to H_2O_2, not H_2O. Using theory, we design and screen the more efficient electrocatalysts toward H_2O_2 synthesis.

- As the single atom catalyst used for H_2O_2 production through an environment friendly way, we test our model catalyst for this reaction. We find TiC supported Au and Pd has higher limiting potential then Pt for H_2O_2 production.

Methane coupling reaction

CO oxidation catalyst

- Based on the first-principles approach, we reports that the ground state geometry of the $Ni@Au_6$ cluster forms chair-like conformation, which is distinctly different from the $Pd@Au_6$ and $Pt@Au_6$ clusters, where hexagonal planar structure is favored over non-planar isomers. The higher stability of the chair like conformation has been verified through various complementary basis sets and methodologies. Further investigations were carried out to show the stability of cluster-assembled material (CAM) based on these small clusters and the CO oxidation reaction was carried out to establish their uses as an industrial catalyst.

Electronic structure of nano-clusters

- Structural and electronic properties of Au_nSn (n = 2–13) clusters are studied by using pseudo potential and LCAO–MO method. A comparison between the structures of Au_n and Au_nSn

clusters reveals that while Au_n clusters favor planar isomers up to n = 13, Au_nSn clusters follow a different trend; 3D structure for n = 3 and 4, quasi planar in the size range n = 5–11, and again 3D isomers from n = 12 onwards. Enhanced contribution of Au p-orbital and significant charge transfer from Sn to the gold atoms is attributed for such interesting growth pattern of Au_nSn clusters

- We have studied the interaction of an oxygen molecule with small tin clusters (Sn_n, n = 2–6, and 10) using plane wave based pseudo-potential method followed by the LCAO–MO approach. The interaction of oxygen with small Sn clusters undergoes through dissociative adsorption process. The Sn_2 shows the highest binding with oxygen by releasing 7.13 eV energy. The higher stability of the Sn_2O_2 cluster was further verified by sharp increase in the energy gap between the HOMO and LUMO energy levels and very high ionization potential value. After oxidation of Sn clusters, the O atoms are attached to small number of Sn atoms, which is in line with the previous experiments. We also investigate the interaction of water molecules with small Sn_nO_2 clusters and it dissociates water exothermally with a small reaction barrier.
- We perform a theoretical calculation on structural and electronic properties of passivated rutile $(TiO_2)_n$ quantum dots as a function of the size of the dots. All theoretical studies on TiO_2 quantum dots face the major obstacle in the passivation of surface dangling bonds. In the present work, we provide a simple passivation way to passivate these clusters, by passivating the surface Ti atoms with –OH groups and surface oxygen atoms with –H. Our study reveals that the HOMO densities for rutile quantum dots are delocalized throughout the whole cluster while that of LUMO are strongly localized on a few surface Ti atoms.

Computer Proficiency:

Operating Systems: Unix/Linux, Windows

Utility Package: Latex, MS/Open Office

Programming language: FORTRAN, MATLAB

List of publications:

List of publications in journals:

[1]. Gihun Kwon, Dongjae Shin, Hojin Jeong, **Suman Kalyan Sahoo**, Jaeha Lee, Gunjoo Kim, Do Heui Kim, Jeong Woo Han and Hyunjoo Lee. Oxidative Methane Conversion to Ethane on Highly Oxidized Pd/CeO_2 Catalysts Below 400 ˚C. ChemSusChem 2020,13,1–6. (IF=7.96).

[2]. Suman Kalyan Sahoo, Youngjin Ye, Seonggyu Lee, Jinkyu Park, Hyunjoo Lee, Jinwoo Lee, and Jeong Woo Han. Rational Design of TiC-supported Single Atom Electrocatalysts for Hydrogen Evolution and Selective Oxygen Reduction Reactions. **ACS Energy Lett.** 4 (2019) 126-132. (IF=19.003).

[3]. Jiwhan Kim, Chi-Woo Roh, **Suman Kalyan Sahoo**, Sungeun Yang, Jeong Woo Han, and Hyunjoo Lee. Highly Durable Platinum Single Atom Alloy Catalyst for Electrochemical Reactions. **Adv. Energy Mater**. 8 (2018) 1701476. (I.F=25.24)

[4]. Santu Biswas, Anup Pramanik, Tasnim Ahmed, **Suman Kalyan Sahoo**, Pranab Sarkar. Superiority of D–A–D over D–A type of organic dyes for the application in dye-sensitized solar cell. **Chem. Phys. Letts**., 649 (2016) 23. (I.F=2.02)

[5]. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar & Chiranjib Majumder. Is mixed oxide of $Sn_xTi_{1-x}O_2$ more effective for H_2O decomposition? A first Principles Study. **Chem. Phys. Letts**., 633 (2015) 175. (I.F=2.02)

[6]. Sandeep Nigam, **Suman Kalyan Sahoo**, Pranab Sarkar & Chiranjib Majumder. Chair like $NiAu_6$: Clusters assemblies and CO oxidation study by ab initio methods. **Chem. Phys. Letts**., 584 (2013) 108. (I.F=2.02)

[7]. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar & Chiranjib Majumder. Influence of Sn interaction on the structural evolution of Au clusters: A first principles study. **Chem. Phys. Letts.**, 543 (2012) 121. (I.F=2.02)

[8]. Suman Kalyan Sahoo, Sougata Pal, Pranab Sarkar & Chiranjib Majumder. Size dependent electronic structure of rutile TiO_2 quantum dots. **Chem. Phys. Letts.**, 516(2011)68. (I.F=2.02)

[9]. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar & Chiranjib Majumder. Oxidation of tin clusters: A first principles study. **Chem. Phys. Letts.**, 518 (2011) 70. (I.F=2.02)

List of publications in conference proceedings:

[1]. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar, Chiranjib Majumder, "Transition metal dimer on Au (111) surface: A first principle study", **AIP Conf. Proc. 1447**, 473 (2012).

[2]. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar, Chiranjib Majumder, "DFT study of H_2O adsorption on TiO_2 (110) and SnO_2 (110) surfaces", **AIP Conf. Proc. 1512, 292** (2013).

[3]. Sandeep Nigam, **Suman Kalyan Sahoo,** Pranab Sarkar, Chiranjib Majumder, "Adsorption of Eu atom at the TiO_2 anatase (101) and rutile (110) surfaces", **AIP Conf. Proc. 1512,** 290 (2013).

[4]. Sandeep Nigam, **Suman Kalyan Sahoo,** Pranab Sarkar, Chiranjib Majumder, "Platinum atomic wire encapsulated in gold nanotubes: A first principle study", **AIP Conf. Proc. 1591,** 468 (2014).

[5]. Sandeep Nigam, **Suman Kalyan Sahoo**, Chiranjib Majumder, "Interaction of ammonia with semiconducting oxide surfaces", **AIP Conf. Proc. 1942,** 120030 (2018).

Poster Presentations:

[1]. "Adsorption and Dissociation of NH_3 on SnO_2 (110), TiO_2 (110), $Sn_{0.5}Ti_{0.5}O_2$ (110) surfaces" **Suman Kalyan Sahoo**, Sandeep Nigam, Pranab Sarkar, Chiranjib Majumder 4th DAE-BRNS Interdisciplinary symposium on material chemistry (ISMC-2012), December 11-15, 2012, BARC, Mumbai

[2]. "Graphene like Sn_{10} cluster on Au (111) surface : A DFT study" **Suman Kalyan Sahoo**, *Sandeep Nigam, Pranab Sarkar, Chiranjib* Majumder 4th DAE-BRNS Interdisciplinary symposium on material chemistry (ISMC-2012), December 11-15, 2012, BARC, Mumbai

[3]. "Sn_n clusters on MgO (001) surfaces: A DFT study" **Suman Kalyan Sahoo**, Sandeep Nigam, Pranab Sarkar, Chiranjib Majumder 4th DAE-BRNS Interdisciplinary symposium on material chemistry (ISMC-2012), December 11-15, 2012, BARC, Mumbai

[4]. "Interaction of O_2 with deposited transition metal atom: activation to super-oxo state" **Suman Kalyan Sahoo**, Sandeep Nigam, Pranab Sarkar, Chiranjib Majumder Proceeding of Trombay Symposium on Radiation and Photochemistry-TSRP-2012.

[5]. "Tuning the electronic properties of SnO2 (110) surface: A First Principles Study" Snadeep Nigam, **Suman Kalyan Sahoo**, Pranab Sarkar, Chiranjib Majumder Proceeding in ISCANM-II, HRI, Allahabad (2011).

[6]. "Dissociative Adsorption of Oxygen Molecule on Sn_n clusters" **Suman Kalyan Sahoo**, Sandeep Nigam, Pranab Sarkar, Chiranjib Majumder, Proceedings of ISMC-2010, BARC Mumbai

[7]. "Size dependent properties of TiO_2 nanoclusters with density-functional tight-binding" **Suman Kalyan Sahoo**, Sougata Pal, Pranab Sarkar, Chiranjib Majumder, Proceedings of -2010, NISER, Bhubneshwer

Oral Presentations:

[1]. Suman Kalyan Sahoo, & Jeong Woo Han. M/TiC as a single atom elecrocatalyst for HER and ORR reactions: A DFT approach. KIChE Fall Meeting. October 19 - 21, 2016, Daejeon, Korea.

[2]. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar & Chiranjib Majumder. Transition metal dimes on Au(111) surface : A first principle study. 56th DAE Solid State Physics Symposium. December 3-7, 2011, VIT, Chennai, India.

References:

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