

**REQUEST FOR ANNUAL INSTALMENT WITH UP-TO-DATE STATEMENT
OF EXPENDITURE**

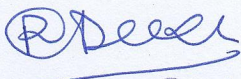
1. Sanction Order No and date: **DST/INT/UK/P-35/2012** Dated: 26.07.2013
2. Total Project Cost: Rs. 23,27,000/-
3. Revised Project Cost: N/A
(if applicable)
4. Date of Commencement: 28.02.2014
5. Statement of Expenditure:

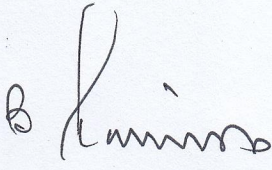
(month wise expenditure incurred during current financial year)

Month & year	Expenditure incurred
February 2014	0.00
March 2014	0.00

6. Grant received in each year:
 - a. 1st Year : Rs. 11,63,500/- (Rupees eleven lakh sixty three thousand five hundred only)
 - b. 2nd Year: : 0.00
 - c. Interest, if any : 0.00

Total (a+b+c): Rs. 11,63,500/- (Rupees eleven lakh sixty three thousand five hundred only)


 03.2015
Prof. Ramesh Ch. Deka
 Department of Chemical Sciences
 School of Science and Technology
 Tezpur University
 Napaam- 784028 : Tezpur : Assam


 Finance Officer
 Tezpur University


 Registrar
 Tezpur University

Statement of Expenditure
(to be submitted financial year wise ie. DOS* to 31st March of that financial year (28-02-2014 till 31.03.2014))

Sr No (I)	Sanctioned Heads (II)	Funds Allocated (indicate sanctioned or revised) Rs. (III)	Funds received Rs. (IV)	Expenditure Incurred I st year (28.02.2014 to 31.03.2014) (V)	Balance as on 31. 03. 2014 (VI)= IV-V Rs.	Remarks (if any)
1	Contingencies	1,00,000	50,000	0.00	50,000	
2	Consumables	6,00,000	3,00,000	0.00	3,00,000	
3(i)	Mobility of scientists For Indian project staff visiting collaborating institute. 4 Visits per year	7,12,000	3,56,000	0.00	3,56,000	
3(ii)	UK project staff visiting Indian collaborating institute: (one number of project staff to undertake project work related visit for 14 man-days in India.) 4 visits each year.	8,80,000	4,40,000	0.00	4,40,000	
4.	Indirect Costs Overhead costs @5% on contingencies/consumables	35,000	17,500	0.00	17,500	
6	Total	23,27,000	11,63,500	0.00	11,63,500	

Ranmath Ch. Deka
Name and Signature of Principal Investigator
Prof. Ranmath Ch. Deka
Department of Chemical Sciences
School of Science and Technology
Tezpur University
Napaam- 784028 : Tezpur : Assam

Date: 19.3.2015

[Signature]
Signature of Competent financial authority
(with seal)

Finance Officer
Tezpur University

Date: 19.03.15

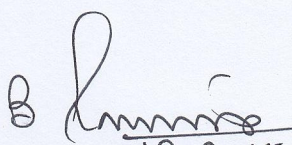
*** DOS – Date of Start of project**

Note :

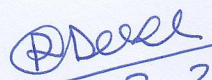
1. Expenditure under the sanctioned heads, at any point of time, should not exceed funds allocated under that head, without prior approval of DST i.e. Figures in Column (VIII) should not exceed corresponding figures in Column (III)
2. Utilisation Certificate (Annexure III) for each financial year ending 31st March has to be enclosed along with request for carry-forward permission to the next financial year.

UTILISATION CERTIFICATE (2 COPIES)
FOR THE FINANCIAL YEAR – 2013-2014

1. Title of the Project/ Scheme: **Hybrid Quantum Mechanics/Molecular Mechanics Calculation on Palladium Supported TiO₂ for CO oxidation**
2. Name of the Institution: Tezpur University
3. Principal Investigator: Dr. Ramesh Ch. Deka
4. Department of Science & Technology sanction order No & date sanctioning the project: DST No: **DST/INT/UK/P-35/2012** Dated: 26.07.2013
5. Head of account as given in the original sanction order: Contingency, Consumables, Mobility of scientists and Overheads
6. Amount brought forward from the previous Financial year quoting DST letter no and date in which the authority to carry forward the said amount was given NA
7. Amount received during the financial year (Please give DST letter/order no and date)
 - i. Amount : 11,63,500/-
 - ii. Letter/Order No: **DST/INT/UK/P-35/2012**
 - iii. Date : 26th July, 2013
8. Total amount that was available for expenditure (excluding commitments) during the financial year (Sr. No. 6+7) Rs. 11,63,500/-
9. Actual Expenditure (excluding commitments) Incurred during the financial year (upto 31st March, 2014) Rs. 0.00/-
10. Balance amount available at the end of the financial year: Rs. **11,63,500/-**
11. Unspent balance refunded, if any (please give details of cheque no etc.): N/A
12. Amount to be carried forward to the next financial year: Rs. 11,63,500/-


 19.3.15
 Finance Officer
 Tezpur University


 Registrar
 Tezpur University


 19-3-2015
 Prof. Ramesh Ch. Deka
 Department of Chemical Sciences
 School of Science and Technology
 Tezpur University
 Napaam-784028 : Tezpur : Assam

UTILISATION CERTIFICATE

Certified that out of Rs 11,63,500/- (Rupees eleven lakh sixty three thousand five hundred only) of grants-in-aid sanctioned during the year 2013-2014 in favour of The Registrar, Tezpur University under this Ministry/ Department letter/ order No **DST/INT/UK/P-35/2012** Dated: 26.07.2013 , no amount was spent during the financial year 2013-2014. The unspent amount of **Rs. 11,63,500 (Rupees eleven lakh sixty three thousand five hundred only)** will be utilized for the next financial year.

Romen C. Dea
Signature of PI

Date *19.3.2015*

B
Signature of Registrar/Signature of Head
Registrar

Date *Tezpur University*

B. L. Manna
Accounts Officer *19.3.15*
of the Institute
Date **Finance Officer**
Tezpur University

(To be filled in by DST)

Certified that I have satisfied that the conditions on which the grants-in-aid was sanctioned have been fulfilled/ are being fulfilled and that I have exercised the following checks to see that the money was actually utilised for the purpose for which it was sanctioned:-

Kinds of checks exercised.

- 1.
- 2.
- 3.
- 4.
- 5.

Signature: _____
Designation: _____
Date: _____

UKIERI DST Thematic Partnership

The report should be completed and submitted jointly by project leaders from India and UK . However separate financial report needs to be submitted by UK and India institutions.

Please complete the report in full and submit by email to
Lakshyata.sinha@britishcouncil.org

UKIERI project details	
Project title	Hybrid Quantum Mechanics/Molecular Mechanics Calculation on Palladium Supported TiO ₂ for CO Oxidation
Project Code	DST/INT/UK/P-35/2012
Names of partner universities/institutions	Tezpur University, Assam, India and University College London, UK
Name of Principal Investigators completing the form	Ramesh Ch. Deka and Richard Catlow
Time Period for reporting	March 2014 to January 2015
Project website/link to social networking page(if applicable)	

Project Statistics	
Number of academic staff involved in & benefiting from related activities	4
Number of students involved in & benefiting from related activities	3

Provide details of staff/student exchange	<ol style="list-style-type: none"> 1. Prof. Ramesh Ch. Deka, Department of Chemical Sciences, Tezpur University, Napaam, Tezpur – 784 028, Assam India. 2. Prof. Richard Catlow, University College London, UK 3. Dr. Andrew Logsdail, UCL 4. Dr. Scott Woodley, UCL
Details of PhD students	<ol style="list-style-type: none"> 1. Mr. Debajyoti Bhattacharjee, Tezpur University 2. Ms. Subhi Baishya, Tezpur University 3. Ms. Pakiza Begam, Tezpur University

Project Outreach and Impact	
Number of research papers published in national & international journals	3
Title of paper	Catalytic Activities of Au ₆ , Au ₆ ⁻ , and Au ₆ ⁺ Clusters for CO oxidation: A density functional study, <i>Int. J. Quant. Chem.</i> 114 , 1559-1566 (2014)
	Catalytic Activity of Anionic Au-Ag Dimer for Nitric Oxide Oxidation: A DFT Study, <i>New. J. Chem.</i> , DOI: 10.1039/C4NJ01328J
	A theoretical insight on NO adsorption on neutral and charged Pd _n (n=1-5) clusters, <i>Int. J. Quant. Chem.</i> (under review)
Date of publication	2014
	2015

Journal (Volume / Number)	Int J Quant Chem, 114 (22); New J Chem (DOI: 10.1039/C4NJ01328J)
No of citations of these papers	1
Media Coverage (newspaper, magazine articles, newsletters etc.)	The visit of Prof. Catlow to Tezpur University was published in leading news papers like Assam Tribune, Amar Asom, Dainik Asom etc. on 22 nd January, 2015.
Could these publications be made available for UKIERI communications?	YES
Has the project received funding from any other source? Provide name of funding body / company sponsoring the project. Mention both India and UK	NO
Amount in GBP/INR	Rs. 23,27,000/- (for Indian partner)
Please provide details of any additional sources of support in cash or in kind	N/A

PROJECT OUTCOMES

1. Please detail your progress against the objectives stated in the proposal (from your Work plan, Outcomes and exchanges section in the Proposal). 400 words

Progress of the Work

Ramesh Ch. Deka, Subhi Baishya, Pakiza Begum and Debajyoti Bhattacharjee

Department of Chemical Sciences, Tezpur University, Assam, India

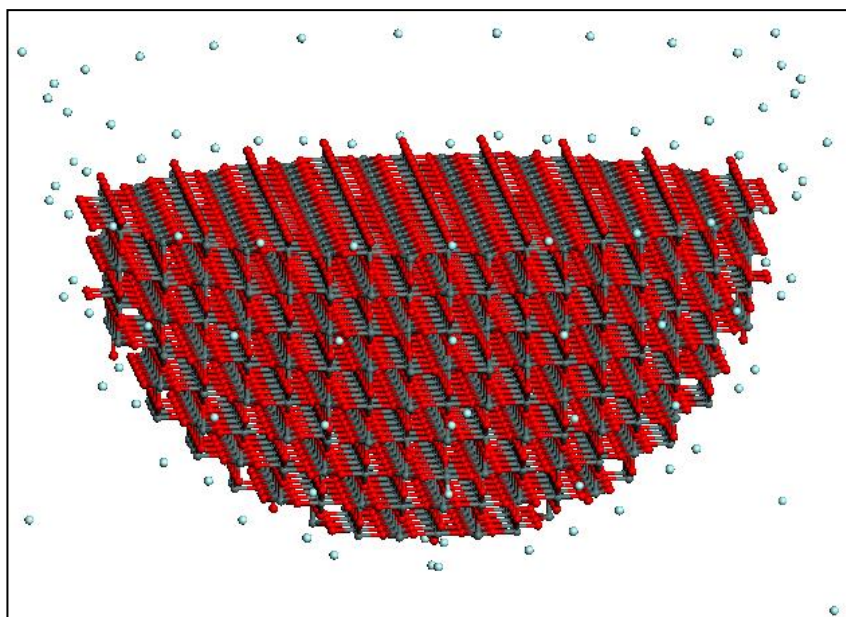
C. Richard A. Catlow, Andrew Logsdail and Scott Woody,

Department of Chemistry, University College London, UK

Our main work focused on catalytic study of bare and metal oxide supported nanoclusters using computational methods. In this regard, the mechanistic details of C-H activation of methane over faujasite supported Au metal were studied in due course. Hybrid quantum mechanics/molecular mechanics method was implemented to study the mechanistic details using GULP code. The main aim of this work was to study the conversion of methane to a value added product-methanol. The oxidation process from methane to methanol proceeds via a pathway involving three transition states-first is the detachment of one hydrogen of methane, second is the formation of OH and third one is the formation of CH₃OH during the reaction. Our results revealed that faujasite supported gold can effectively catalyzed the oxidation of methane.

One important feature that distinguishes clusters from the bulk is the interesting property that their structures can change abruptly with the addition of a single atom. Thus, determination of the global minimum structures of the higher size clusters has become one of the forefronts of the current day research. Therefore, using the collaboration between UCL and Tezpur, we have implemented KLMC code within the GULP interface to generate various starting geometries for gold clusters such as Au₁₆ and Au₂₅. Our calculations generated 20 different isomers which will be further optimized without symmetry constraint using density functional theory in the DMol³ program.

The catalytic activity of metal clusters adsorbed on oxide surfaces can be explored systematically by using model catalysts. Therefore, we construct a parabolic shaped surface of SnO₂ with 3359 atoms. On the oxide surface we anchored a single palladium atom on top of which we studied the adsorption properties a CO molecule using hybrid quantum mechanical/molecular mechanical (QM/MM) simulations in the ChemShell



program package. The adsorption of CO is a fundamental process in CO oxidation.

Fig. Optimised structure of SnO₂ surface.

Considering the wide use of metal oxide nanoclusters in catalysis, we have studied the structure, electronic properties and stabilities of manganese oxide nanoclusters by using global optimization method and DFT. For the global optimization, we have used the KLMC code developed by *Woodley et al* of UCL. Our study targeted on Mn_mO_m clusters with m=1-12. After global optimization we have obtained different geometries for a particular cluster and choose the most stable one for further DFT calculations. The DFT calculations are carried out using DMol³ code. Spin unrestricted calculations are carried out using DNP basis set and BLYP functional for different possible spins of the oxide clusters. This work is still under process. But from the DFT study of the clusters for m=2 and 3, it reveals that strong antiferromagnetic coupling are present in the MnO clusters.

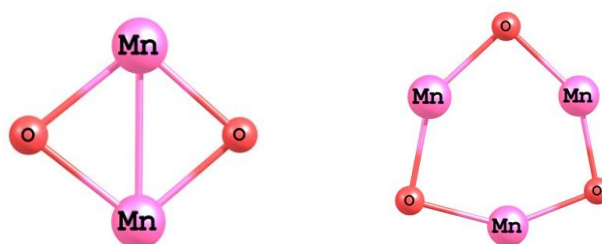


Fig. Global optimized structures for Mn₂O₂ and Mn₃O₃

List of Publications:

1. D. Bhattacharjee, B. K. Mishra, A. K. Chakrabarty and R. C. Deka, *New. J. Chem.*, DOI: 10.1039/C4NJ01328J.

2. P. Begum, P. Gogoi, and R.C. Deka, *Int. J. Quant. Chem.* (Under Review)
3. S. Baishya and R. C. Deka, *Int. J. Quant. Chem.* **114**, 1559-1566 (2014).

Exchange Visits:

To date there have been the following three visits:

1. Prof. Ramesh Ch. Deka visit to UCL (27.04.2014 to 03.05.2014)
 2. Prof. Ramesh Ch. Deka, Subhi Baishya, Pakiza Begum and Debajyoti Bhattacharjee visit to UCL (15. 06.2014 to 06.07.2014)
 3. Prof. Richard Catlow and Dr. Andrew Logsdail visit to Tezpur University (18.01.2015 to 23.01.2015)
2. Financial performance against expenditure in the proposal. Please provide information in the attached spreadsheet against the planned and actual expenditure and any comments. Also mention the commitment of funds for the coming year. The sheet should be authorised by the delegated authority in Finance/research department of the Institution/College/University.
 3. Review of progress towards the achievement of the UKIERI objectives – Long term sustainability, Mutuality and Complementarity, Inclusion and Capacity Building

We are jointly work on reaction mechanisms of CO oxidation, NO oxidation and methane oxidation using metal nanoclusters supported in zeolites and metal oxides. These works are helping in developing trained man power for performing high quality research particularly to the Indian counterpart. Thus this UKIERI scheme will help in achieving long term sustainability and capacity building.

4. Involvement with corporate sponsors outside the UKIERI programme. Are there any organisations or companies involved in the project which are assisting with the funding? N/A
5. Please provide narrative detail on any particular success stories/highlights .

Molecular modelling and quantum chemical software like GULP, KLMC, NWChem, GAMESS-UK, ChemShell etc. have been installed with the UK partners at Tezpur

University, Assam, India.

6. Please provide detail on the impact of project activities to date and evidence used to measure this, particularly with regard to the collaboration.

With the help of this collaborative project following activities are carried out at Tezpur University:

- i. QM/MM calculations for zeolite have been set up and used for catalysis purpose.
 - ii. ChemShell QM/MM calculations are performed for SnO₂ surface.
 - iii. Oxidations of CO, NO and methane have been performed in Au, Pd and Pt supported zeolites.
7. Issues arising from the UKIERI process which can be used as lessons learned for improvement in the future. N/A

Ramesh Ch. Debsa

Signature of Lead PI (India/UK)

(Online submission of report will be taken as signed off copies)

Notes

- UKIERI team may use information from the report for further dissemination of the project as a whole.
- The financial sheet needs to be signed off by a delegated authority from Finance department from the institution/College/University

1. The Assam Tribune, 22nd January, 2015

Tezpur University celebrates 22nd foundation day

CORRESPONDENT

TEZPUR, Jan 21 – The 22nd foundation day of Tezpur University was celebrated with a day-long programme today. Established on this day in 1994, the Central university began its journey with 57 students in three departments, and today it is an institution of reckoning with 3,300 students and 260 faculty members in 19 departments, supported by nearly 300 technical and administrative staff. The university has already awarded various undergraduate and postgraduate degrees to over 6,000 students, including 351 PhD degrees.

Inaugurating the foundation day celebration, Vice Chancellor Prof Mihir K Chaudhuri said that although the university had achieved in the field of academics and extracurricular activities at national and international events in recent times, it has much more to do. Indicating India's importance at the international forum in manpower, he said that in 2016, according to a research group, every fourth skilled manpower would be an Indian.

Prof Arup Kumar Raychaudhuri of the Subhash Chandra Bose National Centre for Basic Sciences, Kolkata delivered the first Foundation Day Oration on 'Innovation and Invention: Lessons from Materials', while Prof Richard Catlow of the University College of London delivered the Second Oration on 'Materials, Molecules and Modelling'. Prof Catlow also highlighted the opportunities available for collaboration between Indian and British universities and various agencies, like the Royal Society and the British Council.

On the occasion, the students who participated at various regional and national events and brought laurels to the university, including the teams winning the 'Sweden-India National Quiz Competition 2014', winners of gold, silver and bronze medals at the 30th Inter-university East Zone Youth Festival, regional winners of the Great Debate 2014 instituted by the British Embassy and other academic and co-curricular activities, were awarded certificates of appreciation. The university also recognized 15 Group B and C employees with the best performance awards.

2. Amar Asom, 22nd January, 2015

তেজপুৰ বিশ্ববিদ্যালয়ৰ প্ৰতিষ্ঠা দিৱসত লণ্ডন বিশ্ববিদ্যালয়ৰ অধ্যাপক ৰিচাৰ্ড কেটল

ষ্টাফ ৰিপ'ৰ্টাৰ, তেজপুৰ, ২১ জানুৱাৰী : তেজপুৰ বিশ্ববিদ্যালয়ৰ ২২সংখ্যক প্ৰতিষ্ঠা দিৱসত আজি বিখ্যাত বিজ্ঞানী তথা কলিকতা নেতাজী সুভাষ চন্দ্ৰ বসু প্ৰতিষ্ঠানৰ অধ্যাপক অৰূপ কুমাৰ বয়চৌধুৰীয়ে আইকন যুগৰ পৰা চিলিকন যুগলৈ বিজ্ঞানে অৰ্জন কৰা সফলতা ব্যাখ্যা কৰি বিজ্ঞানৰ জয়যাত্ৰাৰ অংশীদাৰ হ'বলৈ ছাত্ৰ-ছাত্ৰীসকললৈ আহ্বান জনায়। উল্লেখ্য, তেজপুৰ নপামত ১৯৯৫ চনৰ ২১ ছেপ্টেম্বৰত মাত্ৰ ৬৭গৰাকী ছাত্ৰ-ছাত্ৰী আৰু তিনিটা বিভাগৰে আৰম্ভ হোৱা তেজপুৰ বিশ্ববিদ্যালয়ে বৰ্তমান তিনি হাজাৰ ছাত্ৰ-ছাত্ৰী আৰু ১৯টা বিভাগৰে পৰিপূৰ্ণ লাভ কৰি নতুন অধ্যায়ৰ সূচনা কৰিছে। অনুষ্ঠানত অধ্যাপক চৌধুৰীয়ে বিভিন্ন ক্ষেত্ৰত সফলতা অৰ্জন কৰা ছাত্ৰ-ছাত্ৰীসকলক মানপত্ৰৰে সন্মানিত কৰে। ইফালে প্ৰতিষ্ঠা দিৱসৰ কাৰ্যসূচীত অংশগ্ৰহণ কৰি ব্ৰিটিছ বিজ্ঞানী তথা University College Londonৰ অধ্যাপক ৰিচাৰ্ড কেটলে শৈক্ষিক উত্তৰণত লণ্ডনৰ কেমব্ৰিজ বিশ্ববিদ্যালয়, অক্সফ'ৰ্ড বিশ্ববিদ্যালয় আৰু University College London-এ আগবঢ়োৱা সুবিধাৰ সম্পৰ্কত উল্লেখ কৰে। তেজপুৰ বিশ্ববিদ্যালয়ৰ আজিৰ এই প্ৰতিষ্ঠা দিৱসত ব্ৰিটিছ বিজ্ঞানীগৰাকীক তেজপুৰ বিশ্ববিদ্যালয়ে গামোচা, চেলেং আৰু স্মাৰকৰে সন্মৰ্শনা জনায়।

তেজপুৰ বিশ্ববিদ্যালয়ৰ ২২ সংখ্যক প্রতিষ্ঠা দিবস উদ্‌যাপন

জিলাৰ বাতৰি দিওঁতা

তেজপুৰ, ২১ জানুৱাৰী : ঐতিহাসিক অসম আন্দোলনৰ ফলস্বৰূপে ১৯৯৪ চনত আছিল দিনটোতে স্থাপন হোৱা তেজপুৰ বিশ্ববিদ্যালয়ৰ ২২ সংখ্যক প্রতিষ্ঠা দিবসৰ কাৰ্যসূচীত আজি বিশিষ্ট অতিথি হিচাপে উপস্থিত হৱাহি লন্ডনৰ ফেল' অৱাৰ্ডে ই উনিভাৰছিটি কলেজ, লন্ডনৰ বসায়ন বিজ্ঞান বিভাগৰ অধ্যাপক, পণ্ডিত ৰিচাৰ্ড কেটল' আৰু কলকাতাৰ এছ এম বোস মেচনেল চেণ্টাৰ ফৰ বেছিক ছয়েসেছৰ অধ্যাপক, বিশিষ্ট বিজ্ঞানী অৰূপ কুমাৰ ৰয়চৌধুৰী। উল্লেখ্য যে পূৰ্বা বিশ্ববিদ্যালয়খনৰ উপাচার্য মিহিকান্তি চৌধুৰীয়ে পতাকা উত্তোলন কৰাৰ পিছত বিষ্ণু ৰাভা প্ৰেক্ষাগৃহত অনুষ্ঠিত হয় প্রতিষ্ঠা দিবসৰ মূল কাৰ্যসূচী। প্রতিষ্ঠা দিবসৰ উদ্‌যাপন সমিতিৰ সভাপতি ডঃ নয়নহীপ ডেকা বৰুৱাৰ আদৰ্শী ভাষণেৰে আৰম্ভ হোৱা অনুষ্ঠানত ভাষণ দি উপাচার্য মিহিকান্তি চৌধুৰীয়ে বিগত সময়ৰ বিশ্ববিদ্যালয়খনৰ ক্ৰিয়াতমিক কাম-কাজসমূহ সন্নিবি কৰে। আনহাতে, বিশিষ্ট অতিথি ৰিচাৰ্ড কেটল'ৱে তেওঁৰ ভাষণত নিজে অধ্যাপনা কৰা শিক্ষানুষ্ঠানখনৰ

কাৰ্য্যথৰা বিস্ত্ৰেয়ণ কৰাৰ লগতে বসায়ন বিজ্ঞানৰ শেহতীয়া আৱিষ্কাৰ আৰু বসায়ন বিজ্ঞানৰ ক্ৰিয়া-কলাপ সন্দৰ্ভত বাখ্যা আগবঢ়ায় বিশ্ববিদ্যালয়খনৰ প্ৰ-উপাচার্য ডঃ অনবজোতি চৌধুৰীয়ে অধ্যাপক অৰূপ কুমাৰ ৰয়চৌধুৰীৰ আৰু ডঃ ৰমেশ চন্দ্ৰ ডেকাই ৰিচাৰ্ড কেটল'ৰ পৰিচিতি দাঙি ধৰে। অৰূপ কুমাৰ ৰয়চৌধুৰীয়ে পদাৰ্থ বিজ্ঞানৰ উন্নয়নৰ বিষয়ে উদাহৰণসহ বিস্ত্ৰেয়ণ কৰাৰ লগতে দেশ' প্ৰযুক্তিৰ উত্তৰণ আৰু পদাৰ্থ বিজ্ঞানৰ উত্তৰণে সম্প্ৰতি কেনেকৈ মানৱ সভ্যতাক আগবঢ়াই নিছে তাৰ বাখ্যা দাঙি ধৰে। এই অনুষ্ঠানতে তেজপুৰ বিশ্ববিদ্যালয়ৰ অসমীয়া অধ্যয়ন কেন্দ্ৰলক্ষ্যে প্ৰকাশিত ডঃ জুৰি দত্ত, ডঃ অৰূপ কুমাৰ নাথ আৰু ডঃ সুৰঞ্জনা বৰুৱাৰ তিনিখন ইংৰাজী গ্ৰন্থ উন্মোচন কৰে বিশিষ্ট অতিথিজনৰ লগতে উপাচার্য আৰু প্ৰ-উপাচার্যই। অনুষ্ঠানত বিশ্ববিদ্যালয়খনৰ ৰাষ্ট্ৰীয়-আন্তঃৰাষ্ট্ৰীয় পৰ্যায়ত বিভিন্ন প্ৰতিযোগিতাত বঁটা লাভ কৰা ছাত্ৰ-ছাত্ৰী আৰু পাকদৰ্শী দ্বিতীয় আৰু তৃতীয় শ্ৰেণীৰ কৰ্মচাৰীক অভিনন্দন জনোৱা হয়। সন্ধ্যা ছাত্ৰ-ছাত্ৰীসকলে বাবেবহুবিধ সাংস্কৃতিক অনুষ্ঠান পৰিৱেশন কৰে।

১ পৃষ্ঠাৰ পৰা

UKIERI PROJECT CLOSURE REPORT

Project Details

Project Title	Hybrid Quantum Mechanics/Molecular Mechanics Calculation on Palladium Supported TiO ₂ for CO Oxidation
Project Reference number	DST/INT/UK/P-35/2012
UK Project Leader	Prof. C. R. A. Catlow
India Project Leader	Prof. Ramesh Ch. Deka
UK Institutions	University College London, UK
Indian Institutions	Tezpur University, Assam, India.
Project Start Date	26.07.2013
Project Completion Date	29 February, 2016
Project Closure Report Submission Date	08 November 2016

Project Closure Report

Contents

1	PROJECT PERFORMANCE.....	4
2	FINANCIAL STATEMENT.....	5
3	IMPORTANT LESSONS LEARNT.....	5
4	SUSTAINABILITY & FUTURE WORK.....	6
5	ADDITIONAL INFORMATION.....	6

1 PROJECT PERFORMANCE

1a. Provide very brief information on the objectives of the project with focus on key five highlights.

1b. Provide specific details of deliverables and outcomes in the table below.

Deliverables included in the Work Plan	Outputs	Milestone and Achievements
Global optimization search of $(\text{SnO}_2)_n$ using KLMC and FHI-aims.	Successfully investigated the global optimization search of $(\text{SnO}_2)_n$, $n=1-20$ nanoclusters and study their different structural properties such as band gap, IE, EA, frequency etc.	Manuscript under preparation.
Global optimization search of $(\text{CeO}_2)_n$ using KLMC and FHI-aims.	The global optimization of $(\text{CeO}_2)_n$, $n=1-20$ nanoclusters has also been done successfully and studied different properties.	Manuscript under preparation
An investigation on $(\text{NiO})_n$ $n=2-7$ and their magnetic parameter calculations using KLMC and ORCA program.	Global optimization along with magnetic parameter calculation has been done successfully on $(\text{NiO})_n$, $n=2-7$ and investigated different properties.	Manuscript under communication.
CO oxidation over Au/FAU using ChemShell software	Role of Water on the Adsorption of CO and O ₂ on Zeolite Supported Au Atom: Hybrid Density Functional Theory and Molecular Mechanics Study	Manuscript under preparation
CH ₄ to CH ₃ OH conversion on Pt/FAU using ChemShell Software	Oxidation of methane by atomic oxygen: A QM/MM study	Manuscript under preparation

1c. Provide project statistics in the table below.

Project Statistics	
Total number of faculty directly benefitted through the project and related activities since its inception	4
Total number of faculty benefitted indirectly through the project and related activities since its inception	3

Total number of students benefitted directly through the project and its related activities since its inception (Masters/PhD and Post-Doctoral students)	5
Total number of students benefitted indirectly through the project and its related activities since its inception (Masters/PhD and Post-Doctoral students)	3
Number of any other external individuals/institutes (outside of Partner Institutions) involved in & benefiting from the project or related activities. Please include details of the individuals/institutes.	N/A
Details of staff and student exchanges from the UK to India and India to the UK since inception of the project	<ol style="list-style-type: none"> 1. Prof. Ramesh Ch. Deka visit to UCL (27.04.2014 to 03.05.2014) 2. Prof. Ramesh Ch. Deka, Subhi Baishya, Pakiza Begum and Debajyoti Bhattacharjee visit to UCL (15.06.2014 to 06.07.2014) 3. Prof. Richard Catlow and Dr. Andrew Logsdail visit to Tezpur University (18.01.2015 to 23.01.2015) 4. Prof. Ramesh Ch. Deka, Pakiza Begum and Plaban Jyoti Sarma visit to UCL (11.10.2015 to 26.10.2015). 5. Prof. Richard Catlow and Dr. Andrew Logsdail visit to Tezpur University (18.11.2015 to 25.11.2015). 6. Ms. Pakiza Begum and Mr. Plaban Jyoti Sarma visit to UCL (21.02.2016 to 29.02.2016). 7. Dr Scott M Woodley visit to Tezpur University (21.12.2015 to 27.12.2015)
Any joint agreements/MoUs	Continue the collaboration
Number of PhD Thesis submitted	1
Details of Curriculum development / Course development	Molecular modelling course of Tezpur University has been modified
Details of Train the Trainer modules, resources and actual training beneficiaries	Dr. Subhi Baishya (QM/MM calculations) Ms. Pakiza Begum (Global optimization) Mr. Debajyoti Bhattacharya (Global optimization) Mr. Plaban Jyoti Sarma (Global optimization)

1d. Provide details of project outreach activities.

Project Outreach	
Details of Media Coverage (newspaper, magazine articles, newsletters etc.) with online links or as attachments	The visit of Prof. Catlow to Tezpur University was published in leading newspapers like Assam Tribune, Amar Asom, Dainik Asom etc. on 22 nd January, 2015
Details of additional support from both the institutions in cash and in-kind (Do not mention the in kind support already mentioned in budget proposal)	DST Nanomission
Details of leveraged funding received during the course of the project	SR/NM/NS-1023/2011 (G) dated 3.1.2013 Fund: Rs. 52,93,200
Joint Research papers published in journals (mention title of paper and name of the Journal and no. of citations)	Title of Paper Journal No of citations
Joint Research papers presented at international conference/seminars	Title of Paper: Global Optimization Study of metal oxide nanocluster and Their Application in Catalysis Name of Conference/Seminar : The 6th AICS International Symposium, RIKEN, Japan
Project workshops	Title of the workshop Date /Place No. of participants Relevance of workshop to the project/how did workshop proceeding contribute to project
Any Corporate support to the project in-cash or in -Kind	N/A
Has project work contributed to work of any Corporate/SME	N/A
Has project work led to formation of any SME or creation of jobs? If yes please provide the details	N/A

1e. UKIERI Objectives

Include an evaluation of the project's deliverables against the following criteria to ensure the investment made has been justified

Dissemination and Impact	Knowing the work culture of UK by the Indian students has significant impact in the society as they are the torch bearer of the society. We also learned the art of collaborative research and how quality of research improves through collaboration.
Mutuality and Complementarity	The project gave us an opportunity to visit and exchange our ideas across the table. The Indian team have learned the work culture of UK scientists. The UK scientists also got an opportunity to execute scientific activities through Indian scientists and students and saw how better Indian could do in science.
Contribution to Step Change	N/A
Sustainability	The project was sustainable for long term as nanomaterial research is emerging. After a total visit of eight from both sides we have understand each other and also learned the techniques used in both the laboratories. The focus of India team is to learn the techniques used in ChemShell and KLMC and use the methods in our research for a very long time.
Achievement of Outcomes	We have successfully learned the global optimization technique so called KLMC. We got a solid knowledge on both KLMC and FHI-aims and by applying them in our research work, we successfully studied the structural properties of both $(\text{SnO}_2)_n$ and $(\text{CeO}_2)_n$. where $n=1-20$. As an outcome we have prepared manuscript for both the work and soon we are going to communicate both of them.

1f. PROJECT OUTCOMES

- **Provide details of benefits to UK and Indian Institutions accrued through the project**

During the project we have gain much knowledge on KLMC and ChemShell program. The Indian team got an opportunity to learn ideas and work culture of UK scientists. The UK team saw the India's progress in Science and how better Indian could do in science.

- **Provide details of impact that the output/activity has created or is expected to create**

1. Global optimization search of $(\text{SnO}_2)_n$ using KLMC and FHI-aims. We have Successfully investigated the global optimization search of $(\text{SnO}_2)_n$, $n=1-20$ nanoclusters and study their different structural properties such as band gap, IE, EA, frequency etc.
2. Global optimization search of $(\text{CeO}_2)_n$ using KLMC and FHI-aims. The global optimization of $(\text{CeO}_2)_n$, $n=1-20$ nanoclusters has also been done successfully and studied different properties.
3. An investigation on $(\text{NiO})_n$ $n=2-7$ and their magnetic parameter calculations using KLMC and ORCA program. The global optimization along with magnetic parameter calculation has been done successfully on $(\text{NiO})_n$, $n=2-7$ and investigated different properties.
4. CO oxidation over Au/FAU using ChemShell software. We did detailed study the Role of Water on the Adsorption of CO and O₂ on Zeolite Supported Au Atom. We used a hybrid Density Functional Theory and Molecular Mechanics Study for investigation of different properties of the reaction.

5. CH₄ to CH₃OH conversion on Pt/FAU using ChemShell Software. Oxidation of methane has been done by atomic oxygen. Here we have used hybrid QM/MM study which is very useful for this kind of support system.

2 STATEMENT OF EXPENDITURE

Provide signed-off Statements of Expenditure. These should be in same format as project proposal.

Please note that reports without signed statement of expenditure would be not be accepted.

Statement of Expenditure
(to be submitted financial year wise ie. DOS* to 31st March of that financial year (28-02-2014 till 31.03.2016))

Sr No	Sanctioned Heads	Funds Allocated (indicate sanctioned or revised) Rs.	Funds received Rs.	Expenditure Incurred 1 st year (28.02.2014 to 31.03.2014) (V)	Expenditure Incurred 2 nd year (01.04.2014 to 31.03.2015) (VI)	Expenditure Incurred 3 rd year (01.04.2015 to 31.03.2016) (VII)	Balance as on 31. 03. 2016 (VIII)= IV-(V+VI+VII) Rs.
(I)	(II)	(III)	(IV)				
1	Contingencies	1,00,000	50,000	0.00	19,744	0.00	30,256
2	Consumables	6,00,000	3,00,000	0.00	1,63,115	0.00	136885
3	Mobility of scientists	7,12,000 + 8,80,000 = 15,92,000	3,56,000+4,40,000 =7,96,000	0.00	2,01,819	8,78,201	-2,84,020
4.	Indirect Costs Overhead costs @5% on contingencies/consumables	35,000	17,500	0.00	0.00		17,500
6	Total	23,27,000	11,63,500	0.00	3,84,678	8,78,201	-99379

Ramesh Ch. Deka

Name and Signature of Principal Investigator:
Prof. Ramesh Ch. Deka

Date: 8/11/2016
Department of Chemical Sciences
School of Science and Technology
Tezpur University

* DOS – Date of Start of project
Nacnam-784028 - Tezpur - Assam

Signature of Competent financial authority:
(with seal)

Date: 9.11.16
Finance Officer
Tezpur University

Committed expenditure in the year February 2016 is: Rs. 55,807/-

3. IMPORTANT LESSONS LEARNED

3a. Lessons learned for future reference: We have learned detail about different software like KLMC, FHI-aims and ChemShell. Currently, we are using these methodologies in our research. We are constantly in touch with the UK group and updating our research activities. We are also jointly writing a couple of manuscripts using the KLMC software.

Provide information on any important lessons learned that would be useful for future reference for UKIERI. This could include information on the project approach, the resources, the technology, stakeholders, management organisation structure, management processes and benefits.

3b. Comments on UKIERI

Please include any comments on the UKIERI management process.
Excellent

4. WAY FORWARD

4a. Sustainability

- Provide details on how partnership is going to continue after UKIERI funding is over? (Mention any additional funding already being secured, proposals in pipeline etc.)

We have submitted another proposal to UKIERI for funding and submitting another UK-India joint project from NEWTON Fund.

- Provide details of any future work on this theme

We are planning to use KLMC software for various other metal oxides such as NiO, MgO, MnO etc. The ChemShell software will be used for CO₂ reduction.

- Include details of possible revenue generation mechanism, MOU's joint courses etc.
- **N/A**
- Include details of future opportunities for institutions involved - Sectorial & nationally

**Student exchange
Joint Ph. D. program
Collaborative projects**

- What has been the prosperity benefit through this collaboration to both countries

Work culture, mutual exchange of Ideas

5. Additional Information

Publications:

1. Sarma, P. J., Dowerah, D., Gour, N. K., Logsdail, A. J., Catlow, C. R. A., & Deka, R. C. (2021). Tuning the transition barrier of H₂ dissociation in the hydrogenation of CO₂ to

- formic acid on Ti-doped Sn₂O₄ clusters. *Physical Chemistry Chemical Physics*, 23(1), 204-210.
2. Sarma, P. J., Dey Baruah, S., Logsdail, A., & Deka, R. C. (2019). Hydride pinning pathway in the hydrogenation of CO₂ into formic acid on dimeric tin dioxide. *ChemPhysChem*, 20(5), 680-686.

**REQUEST FOR ANNUAL INSTALMENT WITH UP-TO-DATE STATEMENT
OF EXPENDITURE**

1. Sanction Order No and date: DST/INT/UK/P-35/2012 Dated: 26.07.2013
2. Total Project Cost: Rs. 23,27,000/-
3. Revised Project Cost: N/A
(if applicable)
4. Date of Commencement: 28.02.2014
5. Statement of Expenditure:
(month wise expenditure incurred during current financial year)

Month & year	Expenditure incurred
19-May-14	Rs. 3500
20-May-14	Rs. 17505
21-May-14	Rs. 114333
13-Jun-14	Rs. 2443
25-Jul-14	Rs. 14744
19-Sep-14	Rs. 2165
16-Feb-15	Rs. 82720
25-Feb-15	Rs. 39957
27-Feb-15	Rs. 73461
26-Mar-15	Rs. 5000
26-Mar-15	Rs. 28850
03-Jun-15	Rs. 484163
24-Jun-15	Rs. 69706
06-Nov-15	Rs. 27140
12-Nov-15	Rs. 142300
07-Dec-15	Rs. 60,949
29-Dec-15	Rs. 93,943
Total Amount	Rs. 12,62,879

Grant received in each year:

a. 1st Year : Rs. 11,63,500/- (Rupees eleven lakh sixty three thousand five hundred only)

b. 2nd Year: : 0.00

c. Interest, if any : 0.00

Total (a+b+c): Rs. 11,63,500/- (Rupees eleven lakh sixty three thousand five hundred only)


Finance Officer
Tezpur University

Statement of Expenditure
(to be submitted financial year wise i.e. DOS* to 31st March of that financial year (28-02-2014 till 31.03.2016))

Sr No (I)	Sanctioned Heads (II)	Funds Allocated (indicate sanctioned or revised) Rs. (III)	Funds received Rs. (IV)	Expenditure Incurred 1 st year (28.02.2014 to 31.03.2014) (V)	Expenditure Incurred 2 nd year (01.04.2014 to 31.03.2015) (VI)	Expenditure Incurred 3 rd year (01.04.2015 to 31.03.2016) (VII)	Balance as on 31.03.2016 (VIII)= IV-(V+VI+VII) Rs.
1	Contingencies	1,00,000	50,000	0.00	19,744	0.00	30,256
2	Consumables	6,00,000	3,00,000	0.00	1,63,115	0.00	136885
3	Mobility of scientists	7,12,000 + 8,80,000 = 15,92,000	3,56,000+4,40,000 =7,96,000	0.00	2,01,819	8,78,201	-2,84,020
4.	Indirect Costs Overhead costs @5% on contingencies/consuma bles	35,000	17,500	0.00	0.00		17,500
6	Total	23,27,000	11,63,500	0.00	3,84,678	8,78,201	-99379

Ramesh Ch. Deka
Name and Signature of Principal Investigator:
Prof. Ramesh Ch. Deka
Department of Chemical Sciences
School of Science and Technology
Tezpur University
Napaam 784020, Tezpur, Assam
Date: 8/11/2016
* DOS - Date of Start of project

B. Kumar
Signature of Competent financial authority: _____
(with seal) 3/12/16
Finance Officer Date: _____
Tezpur University

Committed expenditure in the year February 2016 is: Rs. 55,807/-

UTILISATION CERTIFICATE (2 COPIES)
FOR THE FINANCIAL YEARS – 2014-2015 and 2015-2016

1. Title of the Project/ Scheme: **Hybrid Quantum Mechanics/Molecular Mechanics Calculation on Palladium Supported TiO₂ for CO oxidation**
2. Name of the Institution: Tezpur University
3. Principal Investigator: Dr. Ramesh Ch. Deka
4. Department of Science & Technology sanction order No & date sanctioning the project: DST No: **DST/INT/UK/P-35/2012** Dated: 26.07.2013
5. Head of account as given in the original sanction order: Contingency, Consumables, Mobility of scientists and Overheads
6. Amount brought forward from the previous Financial year quoting DST letter no and date in which the authority to carry forward the said amount was given NA
7. Amount received during the financial year (Please give DST letter/order no and date) i. Amount : 11,63,500/-
ii. Letter/Order No:
DST/INT/UK/P-35/2012
iii. Date : 26th July, 2013
8. Total amount that was available for expenditure (excluding commitments) during the financial year (Sr. No. 6+7) Rs. 11,63,500/-
9. Actual Expenditure (excluding commitments) Incurred during the financial year (upto 31st March, 2016) Rs. 12,62,879/-
10. Balance amount available at the end of the financial year: Rs. **-99,379/-**
11. Unspent balance refunded, if any (please give details of cheque no etc.): N/A
12. Amount to be carried forward to the next financial year : Rs.Nil/-
13. Actual Expenditure Incurred during the next financial year (upto 31 March, 2016) :Rs. 12,62,879/-


 Finance Officer
 Tezpur University

UTILISATION CERTIFICATE

Certified that out of Rs 11,63,500/- (Rupees eleven lakh sixty three thousand five hundred only) of grants-in-aid sanctioned during the year 2014-2016 in favour of The Registrar, Tezpur University under this Ministry/ Department letter/ order No **DST/INT/UK/P-35/2012** Dated: 26.07.2013. The amount spent during the financial years 2014-2015 and 2015-2016 is Rs. 12,62,879 (Rupees twelve lakh sixty two thousand eight hundred and seventy nine only). The amount of Rs. 99,379/- (Rupees ninety nine thousand three hundred and seventy nine only) which was over spent may release by DST from the sanctioned amount.

Ramesh Ch. Deka
Signature of PI

Date 8/11/2016

Prof. Ramesh Ch. Deka
Department of Chemical Sciences
School of Science and Technology
Tezpur University
Napaam- 784028 : Tezpur : Assam

B
Signature of Registrar/Signature of Head
Registrar
Tezpur University

Date

B K
Accounts Officer
of the Institute
Date 8/11/16
Finance Officer
Tezpur University

(To be filled in by DST)

Certified that I have satisfied that the conditions on which the grants-in-aid was sanctioned have been fulfilled/ are being fulfilled and that I have exercised the following checks to see that the money was actually utilised for the purpose for which it was sanctioned:-

Kinds of checks exercised.

- 1.
- 2.
- 3.
- 4.
- 5.

Signature: _____
Designation: _____
Date: _____