



INDO-KOREA SCIENCE & TECHNOLOGY CENTER

**BI-ANNUAL
REPORT**
2015 and 2016

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KIST

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TECHNOLOGY CENTER

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KIST

INDO - KOREA SCIENCE & TECHNOLOGY CENTER

ಇಂಡೋ-ಕೊರಿಯ ಸೈನ್ಸ್ ಅಂಡ್ ಟೆಕ್ನಾಲಜಿ ಸೆಂಟರ್

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VISION STATEMENT

“Establish a Global Knowledge Platform that would bring together technologists and scientists across academia and industries in Korea and India to foster creative and innovative research to solve complex and challenging problems that would impact the society at global level.”



From the Desk of the Director
3

*Evolution of Indo-Korea
Science & Technology Center*
5

The Organization
11

Research
17

Activities
35

From the Desk of the Director

In 1966, the Korean government established *Korea Institute of Science and Technology* (KIST) to develop the technologies required for industrial growth. The establishment of KIST allowed Korea to lay the foundation for a modern Science and Technology (S&T) capacity and infrastructure when no meaningful industry in the modern sense existed. KIST became the prime model for specialized research institutes that began to spring up in the mid-1970s. Over these 50+ years, with KIST's able leadership, R&D infrastructure and technology development capacity have rapidly expanded in all areas of research in Republic of Korea.



Dr. Seung-Cheol Lee
DIRECTOR

Both Korea and India have always used S&T as an instrument for achieving socio-economic good. Bilateral ties between Korea and India have progressively been upgraded through strategic partnership in several areas. In 2010, KIST established *Indo Korea Science and Technology Center* (IKST) with the following objectives:

1. To establish collaboration between reputed Korean and Indian research institutions for building an environment of enriched cooperation and provide an eco-system for smooth interconnectivity.
2. To establish an efficient system for exchange of scientists and researchers between Korea and India.
3. To work closely with industry, especially small and medium scale ones, to resolve some of their technology issues in specific domains through industry-research partnership between Korea and India.



Since 2015, apart from forming a small team of committed researchers drawn from industry and research institutions for its internal research, IKST also signed Memoranda of Understanding (MOU) with reputed research institutions like *Jawaharlal Nehru Centre for Advanced Scientific Research* (JN-CASR), autonomous universities like *Christ University* (CU), and State government agencies like the *Karnataka Science & Technology Academy* (KSTA) to achieve its objectives.

This report briefly covers research activities that are going on at IKST, both internally as well as in collaboration with some of the Indian research / academic institutions. Every year IKST also either independently or in association with other institution(s) conducts workshop / seminar / technology forum for exchanging / disseminating knowledge as well as to build networks. This report also covers a brief note on such workshops or seminars conducted by IKST.

As stated in its vision, IKST endeavours to establish a Global Knowledge Platform (GKP) that would bring together scientists and researchers in Korea and India to build a strong network to address some of the complex and challenging issues facing the world in general, Korea and India in particular.

Evolution of Indo-Korea Science & Technology Center

Science and Technology (S&T) has been a priority in the Republic of Korea for over five decades. The country's rapid economic transformation, often called the 'Miracle of Han river', is the result of large investments made into S&T by successive governments. Korean GDP grew from US\$ 2.7 billion in 1962 to US\$ 230 billion in 1989. Korea has been investing more than 4% of its GDP in R&D, a fact which has made it one of the highest spenders of R&D in the world.



Dr. M V Ravikumar

ADVISOR

Korea and India are progressively upgrading their bilateral relationship through strategic partnerships for over a decade. During February 2006 as part of Comprehensive Economic Partnership Agreement, Dr. D. H. Kunn, then President of *Korea Institute of Science and Technology* (KIST) signed a Memorandum of Understanding (MOU) with Dr. Rajiv Sharma, Advisor & Head, International Cooperation, *Department of Science & Technology* (DST), Government of India, to develop further cooperation in the field of prospective technologies for the common benefit of two countries. Based on this MOU, KIST entered into an agreement with the *Indian Institute of Science* (IISc.) during July 2006 to undertake collaborative research between their researchers.

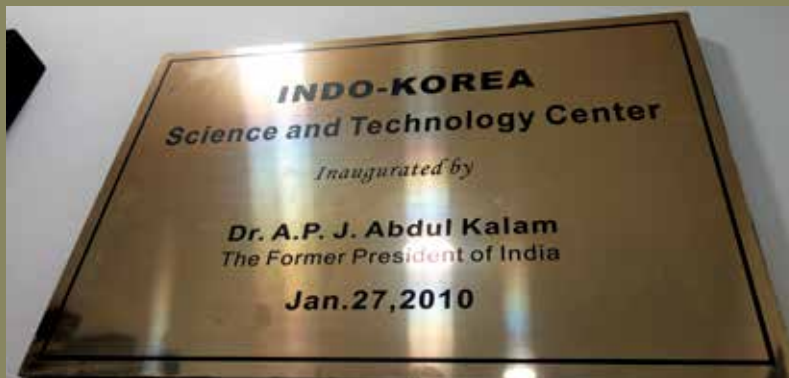
During 2007, then President of India, Dr. A. P. J. Abdul Kalam during his visit to Korea held talks with then Presidential candidate Dr. Lee Myeong-bak for establishing a *Global Knowledge Platform* (GKP) through which some of the successful technologies could be used for developing rural India, thus bringing the two countries closer. Subsequently Dr.



Kalam participated in the Presidential Inauguration ceremony of Dr. Lee Myeong-bak during February 2008 and further strengthened the ties between the two countries. The first GKP workshop was conducted in Korea during August 2008 in the areas of materials science, renewable energy, water and environment.

In December 2009, an agreement was signed between KIST and IISc. to establish the KIST-IISc. Cooperation Center, named as *Indo Korea Science and Technology Center* (IKST) in the IISc. campus with the main objective of strengthening on going collaboration between the two institutions and establish GKP. During January 2010, IKST was formally inaugurated by former Indian President Dr. A. P. J. Abdul Kalam in the presence of Dr. Ahn Byeong-man, Hon. Minister of Education, Science and Technology, Republic of South Korea; Dr. Min Dong-pil, Director of KRCF; Dr. Han Hong-taek, Director of KIST; Dr. Balaram, Director, IISc.; Dr. Balakrishnan, Associate Director of IISc. and Dr. Rajiv Sharma, Advisor and Head, International Cooperation, DST.

Apart from strengthening collaboration between KIST and IISc. initially, IKST was focusing on finding suitable industry partners for adopting some of the successful technologies developed by KIST and other Korean Research institutions in the areas of energy, water & sewage and robotics by jointly hosting 'Technology Forums' in partnership with DST, Research / Academic institutions and Indian Industries' Association.

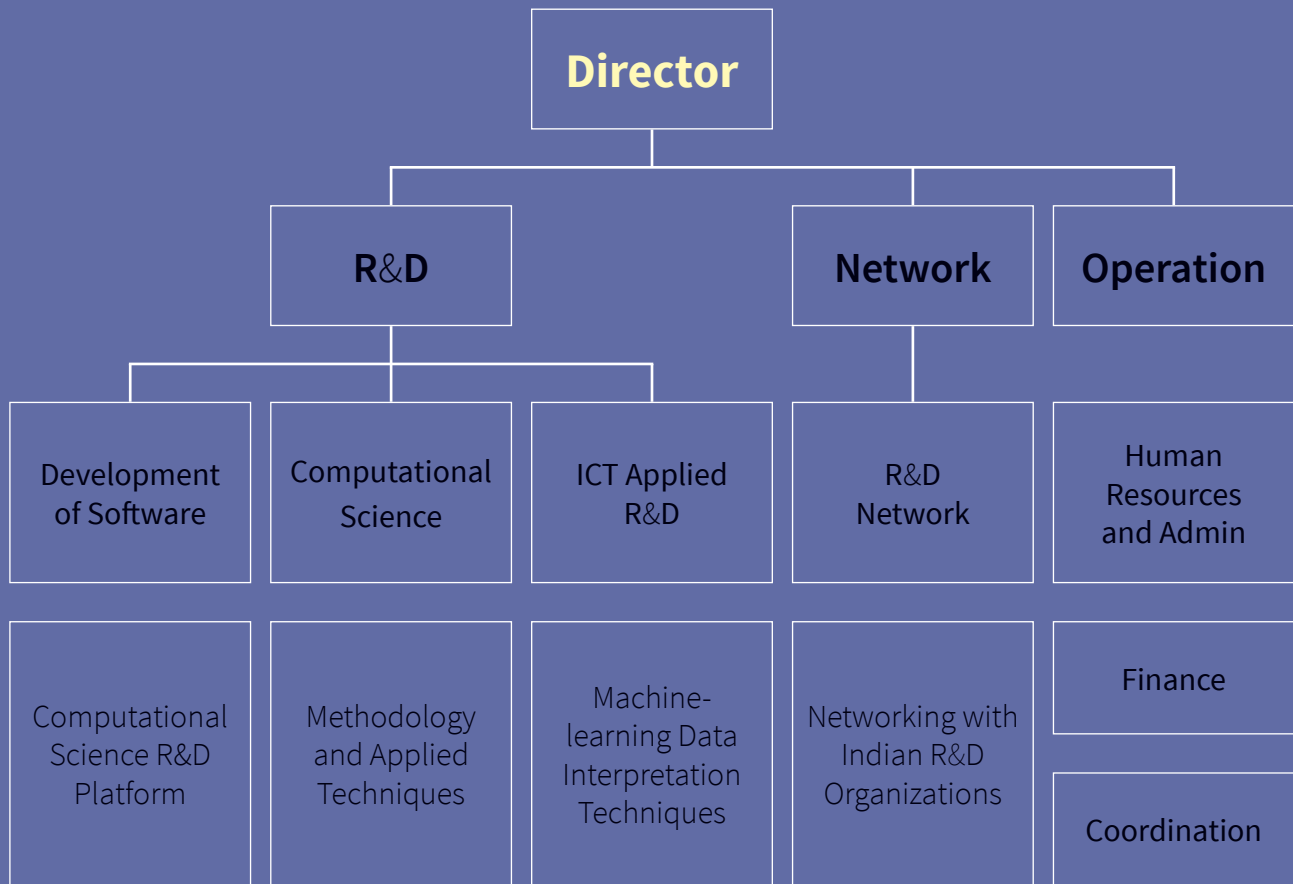


During October 2013, KIST signed an MOU with the *International Center for Materials Science*, established at *Jawaharlal Nehru Centre for Advanced Scientific Research* (JNCASR). KIST deputed a Senior Research Scientist Dr. Seung-Cheol Lee to establish collaborative research program with JNCASR in the area of computational science. As then director of IKST resigned during October 2014, Dr. Lee was requested to officiate as director. During 2015 there was transition in the Board of Directors of IKST and also focus was changed to more on collaborative projects and internal research program. IKST moved to an independent office outside IISc. closer to its MOU partner JNCASR during August 2015 and signed up fresh MOUs with Karnataka Science and Technology Academy, Government of Karnataka to explore possibility of identifying more research partners. IKST has also signed an MOU with *Christ University* for conducting joint workshop, forums to establish industry-research initiatives. Having developed its own 'Vision-Mission' plan, currently IKST is building network with some of the reputed Indian Research institutions to work with Korean Research institutions in general and KIST in particular.

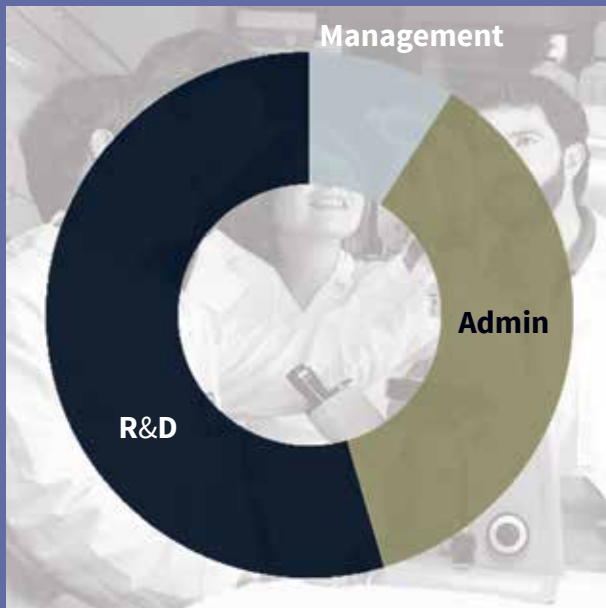


The Organization

Organization Chart

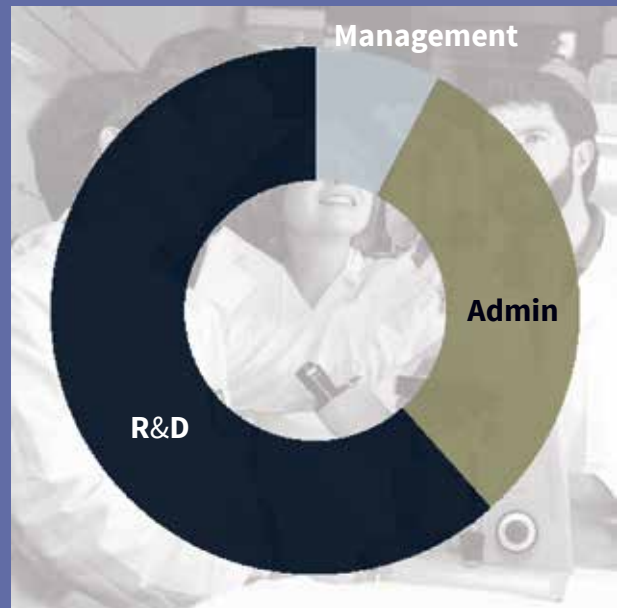


Manpower 2015



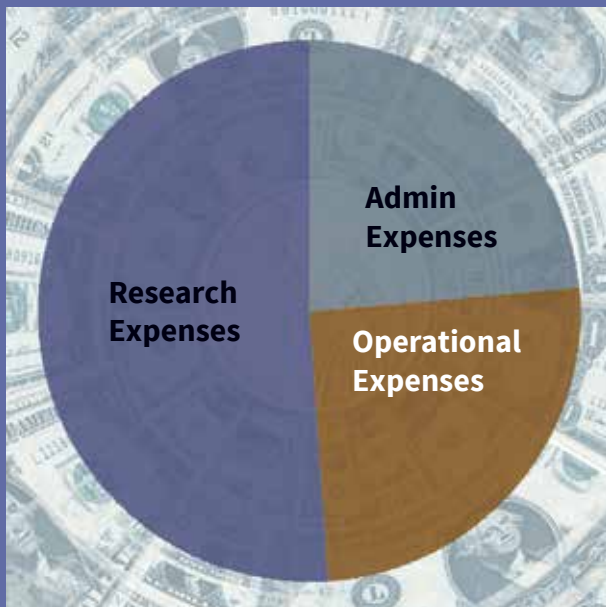
Management **9.1%** (1 of 11)
Admin **36.4%** (4 of 11)
R&D **54.5%** (6 of 11)

2016



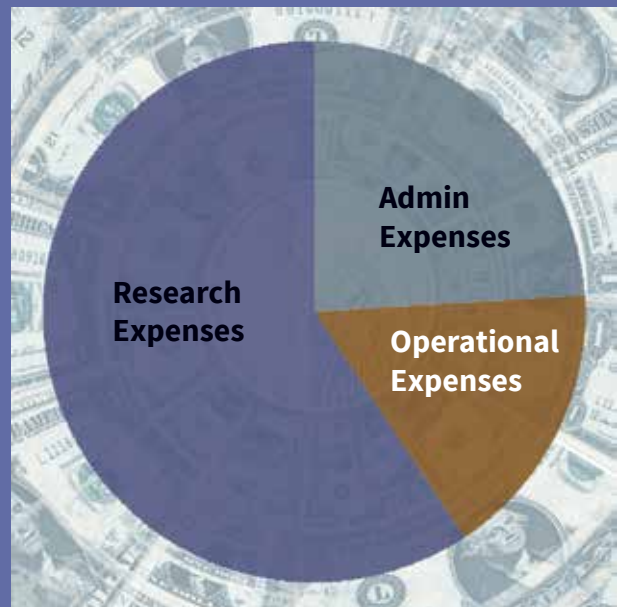
Management **7.7%** (1 of 13)
Admin **30.8%** (4 of 13)
R&D **61.5%** (8 of 13)

Funds Deployed 2015



Admin expenses **23.6%**
Operational expenses **25.3%**
Research expenses **51.1%**

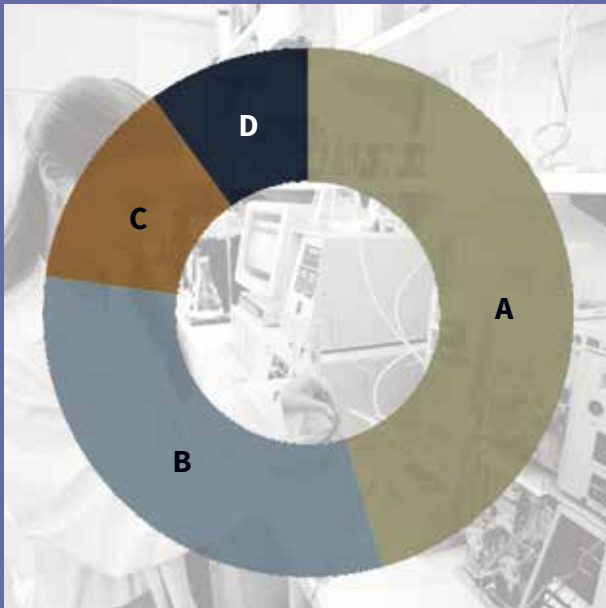
2016



Admin expenses **24%**
Operational expenses **16.7%**
Research expenses **59.3%**

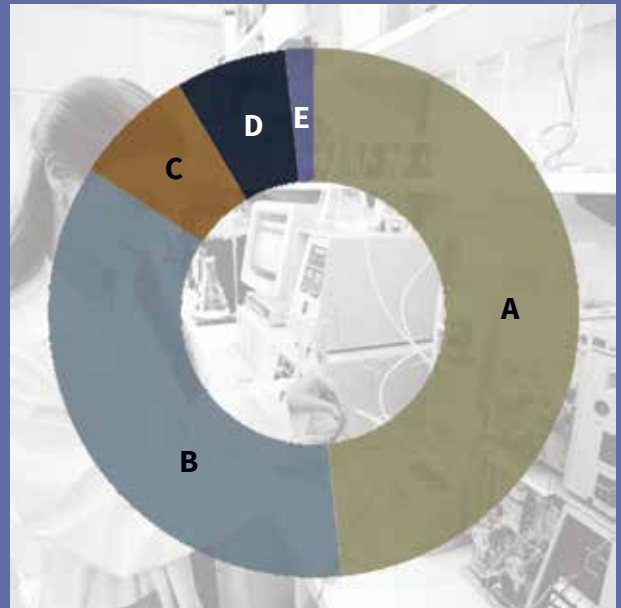
Research Funds

2015



A. Outsourced Project **46%**
 B. Collaborative Project **32%**
 C. Internal Project **12%**
 D. Workshop & Seminar **10%**

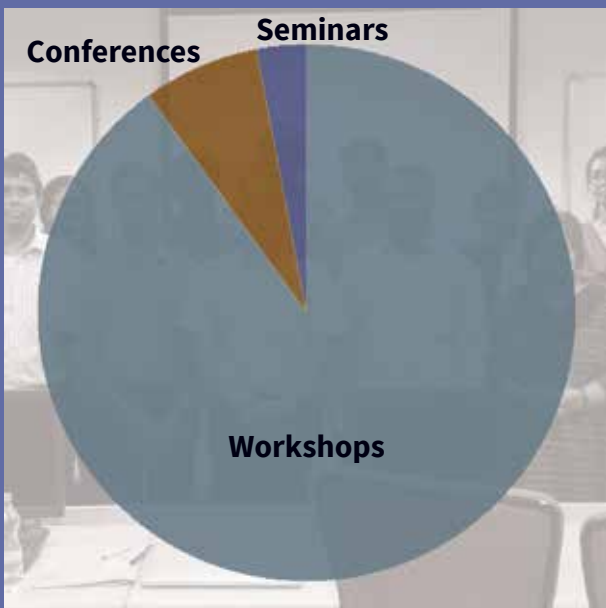
2016



A. Outsourced Project **48.3%**
 B. Collaborative Project **35.8%**
 C. Internal Project **7.4%**
 D. Workshop & Seminar **6.8%**
 E. HR Exchange Program **1.7%**

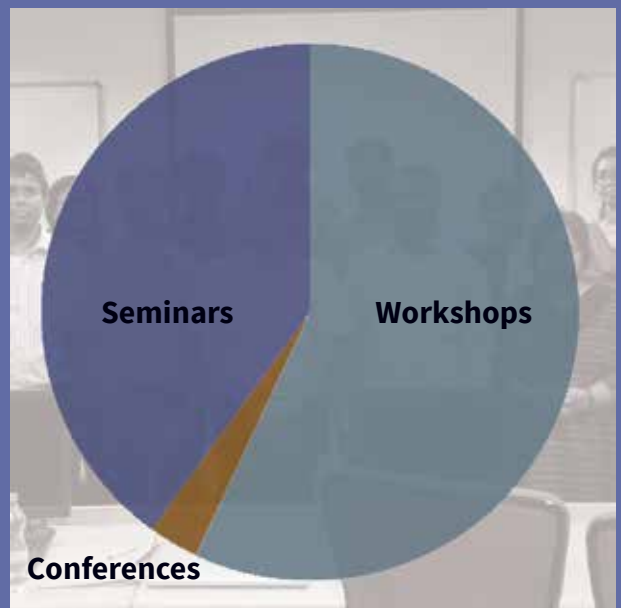
Activities

2015



Workshops **90%**
 Conferences **7%**
 Seminars **3%**

2016



Workshops **57%**
 Conferences **3%**
 Seminars **40%**



Research

Machine Learning *abinitio* configuration energies of a multi- component solid solution



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Introduction

The question that confronts anyone attempting to model solid solutions at atomic scale using *abinitio* or first-principles methods, such as those based on density functional theory (DFT), is the choice of configuration. More precisely, among the large number of possible configurations which is the most-likely configuration that the system would choose to be in, or in other words, what is the most-likely lowest energy configuration of atoms? Answer to this question is crucial since the atomic configuration is an input to DFT calculations, and hence, this information is required *a priori*. Such a question has definitive answer for ordered crystalline materials since the ground state configuration is well separated by the next higher-energy configuration, which ensures that all the atoms occupy ordered lattice positions each time the material is synthesized. As an example, Ni_3Al crystallizes in $L1_2$ structure, a face-centered cubic (FCC) lattice with Al at corners and Ni occupying face-centered positions. The unique ground state configuration in ordered

crystalline materials makes life simpler while performing DFT calculations. Unfortunately this comfort is missing for solid solutions since atoms are distributed randomly on the lattice sites. This gives rise to a large number of configurations very close to the “ground state” (even if existence of such a state is not known), and the system crystallizes randomly into any one of them during synthesis.

Absence of *a priori* information of low-energy configuration poses a computational challenge in *abinitio* modeling of solid solutions. Over the years, methods have been developed to address this problem, primarily following two routes. The first route is based on combining DFT calculated energies for select configurations with statistical mechanics using cluster expansion (CE) [1,2]. The CE-based approach also enables calculation of configurational free energy at finite temperatures, and have been used extensively to study phase diagrams of binary alloys. Recently, CE was used to model partitioning of elements between γ and γ' in a 4-component Ni-based alloy [3]. The second route to model solid solution is based on special quasi-random structures (SQS), constructed to approximate radial distribution function of an ideal solid solution [4]. The SQS becomes a direct input to DFT to calculate thermophysical properties.

Despite much progress, performing *abinitio* calculations for realistic solid solution alloys is still beyond the reach of CE and SQS. This is due to the fact that most of the industrially-relevant materials, such as Ni-based superalloys used in gas-turbines and aircraft engines, can contain anywhere between 6 to 9 major elements*. Combinatorial increase in the size of the configurational space with every additional component makes these alloys beyond the reach of known modelling techniques. Recently, a new method based on machine learning has been proposed to address this challenge [5]. Below, essential features of this approach are described.

* Another example is the high entropy alloy (HEA) that can contain > 4 elements in almost equiatomic proportion.

Machine Learning

Methods to unravel hidden pattern and capture correlations between variables in data, thus allowing the user to perform quantitative analysis, broadly defines the domain of machine learning (ML). The ML is based on the premise that given sufficient data, an output quantity (also referred to as target or response variable) can be related to (or modeled by) variables representing the data. ML models does not concern with the underlying physics or mechanism that generated the data; it implicitly encodes that information in the model parameters by building relational dependency between the variables and the output quantity. This domain-independent nature of ML has made it very attractive and led to its widespread use today for constructing classification and regression models in almost all fields where large volume of data is generated. Thus, apart from science and engineering, ML has been applied in finance, social science, consumer, sports, media, business strategy, etc.

The predictive accuracy of an ML model depends on the training algorithm, an appropriate feature set (representing variables), and the input data. If the feature set is represented by $\mathbf{x} \equiv (x_1, x_2, \dots, x_k)$, and the labeled data provided is of the type $(y_1, \mathbf{x}_1), (y_2, \mathbf{x}_2), \dots, (y_k, \mathbf{x}_k), \dots, (y_N, \mathbf{x}_N)$, in its basic form an ML model can be trained to minimize the cost function $S_\theta = \sum_k |y_k - \tilde{y}_k|^2$ where the summa-

tion is over the dataset not used for training and $\tilde{y}_k = f(\mathbf{x}_k; \boldsymbol{\theta})$ is the model-predicted value. Various algorithms have been devised to minimize the cost-function S_θ in the parameter space spanned by $\boldsymbol{\theta}$, and is readily available as standard library in different programming languages. Once the optimized model parameter $\boldsymbol{\theta}_0$ is obtained, it can be used for predicting unlabeled data $\tilde{y}_k = f(\mathbf{x}_k; \boldsymbol{\theta}_0)$.

Machine Learning configuration energy of solid solution

In Ref. [5], it was shown that ML approach, described in preceding paragraph, can be used to accurately model the configurational energy $E(\boldsymbol{\sigma})$ of a multicomponent solid solution alloy if the model is trained with $E_{DFT}(\boldsymbol{\sigma})$, calculated for a set of random configurations. The crucial factor in constructing ML model of $E(\boldsymbol{\sigma})$ is the feature set which should encode the information on spatial correlation between atoms. This is achieved by using spatial correlation functions, specifically, pair correlation $g^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$ and triplet correlation $g^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ functions (the latter is restricted to equilateral triangle) between all combinations of the alloy components. As an example, for a solid solution of Ni, Al, Ti, Co and Cr, following $g^{(2)}$ is used: Ni–Ni, Ni–Al, Ni–Ti, Ni–Co, Ni–Cr, Al–Al, Al–Ti, Al–Co, Al–Cr, Ti–Ti, Ti–Co, Ti–Cr, Co–Co, Co–Cr, and Cr–Cr; similar combinations of triplet is used to construct $g^{(3)}$. For any configuration

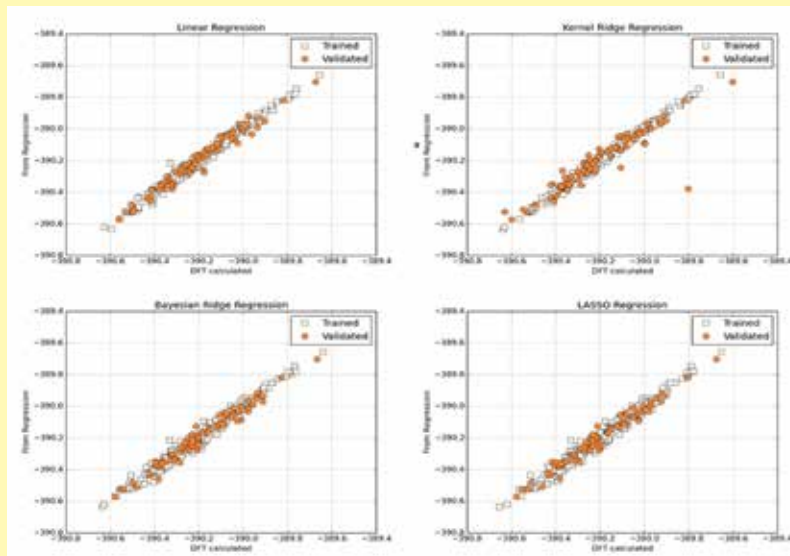


Figure 1 Machine learning predicted configuration energy compared with DFT calculations using four different algorithms for a 64-atom system formed by 8Al–1Co–2Cr–6Ti (rest Ni).

of atoms, these correlation functions, represented by histograms, are concatenated to form a one-dimensional vector $\mathbf{g}$, representing the feature vector for σ – see Ref. [5] for more details.

To demonstrate the capability of ML-based approach, a 64-atoms system with 8Al–1Co–2Cr–6Ti (rest Ni) is chosen. The code was implemented in Python using Scikit-Learn library. Fig. 1 compares the ML predicted configuration energy $E_{ML}(\sigma)$ with its DFT calculated energies $E_{DFT}(\sigma)$; the validated dataset was not used for training. Four different ML algorithms were tested. The training was performed with 240 DFT calculated energies, with 60 energies used for validation. As evident from the plot, ML prediction of $E(\sigma)$ is comparable to the DFT calculated energies with errors < 100 meV (in total energy). The errors could be reduced down to 30meV (in total energy) by increasing the size of the training set.

With ML model of $E(\sigma)$, it is possible to rapidly span the configuration space and generate an accurate distribution of configurational energies $P(E(\sigma))$, as shown in Fig. 2. Further, the $P(E)$ can be used to access specific configurations, such as in low-energy region, for further calculations for material properties and parameters.

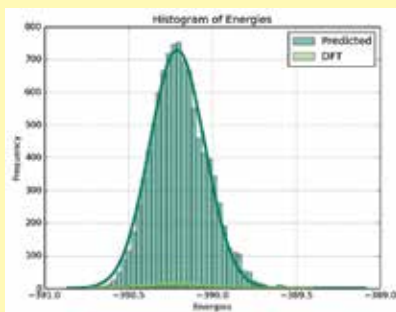


Figure 2 Distribution of configuration energy using ML model; thick line is a fit to normal distribution.

Conclusions and Outlook

The above work shows that machine learning provides an alternative and computationally cheaper approach to modelling multicomponent solid solution alloys at atomic scale. Specifically, it allows one to choose low-energy configurations to perform further calculations which was hitherto not

possible. The method is general enough to be extended to any number of components, limited only by the DFT calculation to generate the training set. The ML-based approach opens up the route to calculate thermomechanical and thermodynamic properties of multicomponent alloy. It also would aid in calculating material parameters of multicomponent alloys required for higher length-scale models, as depicted in Fig. 3.

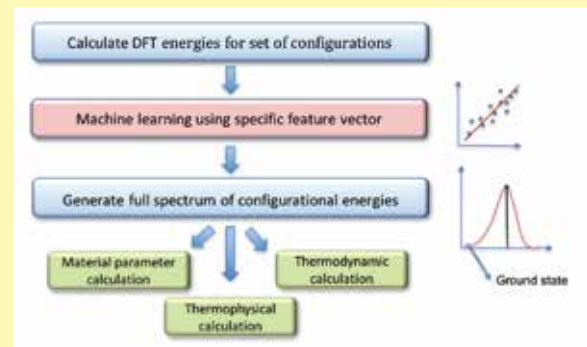


Figure 3 Roadmap for *abinitio* calculation combining density functional theory (DFT) with machine learning.

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First-principles design of efficient, robust catalysts for fuel cell applications



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Introduction

A fuel cell is a device similar to battery and has application as a power source [1]. It can be used as a stationary power source (such as power generating stations) in transport vehicles as well in portable electronic devices (such as mobile, laptop etc.) [2,3]. The fuel cell mainly consists of two electrodes – anode and cathode, coated with catalysts and separated through an ion-conducting electrolyte. Depending on the nature of electrolyte and fuel used, fuel cells are further classified into various types such as solid oxide fuel cell (SOFC), proton exchange membrane fuel cell (PEMFC), direct methanol fuel cell (DMFC), etc. [4]. We are working in close collaboration with experimental groups in Korea on designing efficient catalysts for PEMFC as well SOFC application using first principles methods.

For PEMFC, platinum (Pt) is used as catalyst in both anode and cathode. The electrochemical half-cell reaction that takes place in anode is the *hydrogen oxidation reaction* (HOR) while in the cathode *oxygen reduction reaction* (ORR) occurs. The former reaction is relatively faster and requires small amount of platinum; however, the latter (ORR) is very

slow and requires large amount of platinum loading, since many active cathode sites are lost due to their over-binding to the reaction intermediates and their subsequent accumulation [5,6] on the cathode surface. To circumvent such problem, platinum alloyed with cheap transition metals (M) such as iron, nickel, cobalt, etc., are used. Such alloy (PtM) catalysts show better activity than pure platinum; however, yet activity is much weaker than expected [7]. This is due to the oxidation of the transition metal in the aqueous environment [8]. To address this problem, our research (experimental) colleagues in Korea came up with an idea of modifying the electronic structure of the metal atoms selectively by attaching nitrogen-containing ligand. They developed highly active and durable carbon-supported PtCo alloy nanoparticle (PtCo/C-PNIPAM) using poly N-isopropyl acrylamide (PNIPAM) functionalized carbon (C-PNIPAM) as a support material to selectively modify the surface of the Co atoms [9].

Such hybrid organic-inorganic nanoparticles (a schematic representation is shown in the Fig.1) have been shown to exhibit high electrochemical efficiency and high

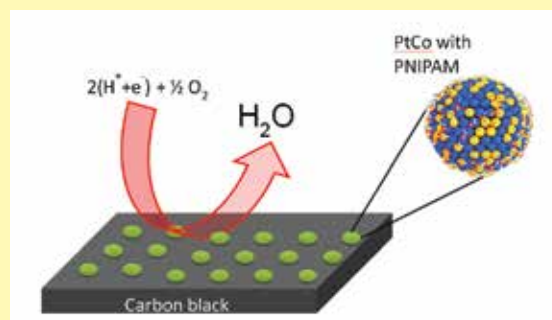


Figure 1 Schematic representation of the CoPt-C/PNIPAM catalyst. Blue balls represent Pt and yellow ones Co.

resistance to erosion. We carried out state-of-the-art quantum mechanical calculations to explain the underlying mechanisms at the atomic scale responsible for the experimental observations, using NH_3 as a model for the nitrogen containing ligand. Enhancing the catalytic activity in this route depends on the choice of the 3d transition metal and the associated ligand to cover it with. The

ligand binding to the 3d transition metal should be stronger than its binding to Pt, so that selective coverage can happen. From the first-principles method, we explored why a ligand prefers to bind to M-sites in PtM alloy, even though its binding to Pt is stronger in elemental form. We analysed the important role played by certain physical parameters – charge transfer, magnetism and strain. Then, we looked more deeply the role played by the magnetism in chemical reactivity of transition metals using an extended d-band centre model.

For the SOFC catalysts, we are working in collaboration with the experimental group of Sejong University in Korea, to design efficient bifunctional catalysts through doping the standard catalysts such as $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Fe}_{0.8}\text{Co}_{0.2}\text{O}_{6-\delta}$ (BSCF).

First principles simulation of the bi-metallic catalysts for PEMFC applications

We performed Density functional theory (DFT) based simulations considering NH_3 adsorbed CoPt as a model system for the PtCo / C-PNIPAM catalyst. Our calculation of adsorption energies show that NH_3 prefers to bind to Co sites than Pt sites. Our calculation of Bader charges also reveals enhancement of charge transfer from Co to Pt due to the surface modifications with N-contained ligands. Such charge transfer pushes the d-band of the Pt to lower energies, resulting less number of blocked Pt-site (due to accumulation of oxygen species) and therefore, enhance overall activity, which was further confirmed by the calculation of Pt-O binding energies which clearly shows that the oxidation and dissolution of the Pt can be prevented through such N-containing ligand treatment. Furthermore, such treatment of ligands on Co sites reduces the possibility of the loss of Co as a vacancy [9].

Continuing further, we studied the origin of strong binding of the nitrogen containing ligand to the 3d transition metal sites in the alloy environment. We found that such preference originates from a combined effect of the charge transfer, magnetism and strain effect [10]. We then quantified the role of each

of them through the calculation of the energy scales associated with them. We studied three bimetals – FePt, CoPt and NiPt; all of them show similar trend in terms their reactivity to NH_3 molecule [11].

Role of magnetism in the chemical reactivity of the transition metals

We then studied extensively the role played by magnetism in the context of transition metal catalysis. For the prediction of the trend of the catalytic behaviour in transition and noble metals, the most widely used *d-band centre* model, which correlates the adsorption energy to the average energy of the d electrons (d band centre) of the metal surface and has proved successful in understanding the chemical bonding in heterogeneous interfaces of various solid-gas and solid-liquid phases [12,13,14]. We demonstrated that this model, which was initially proposed for studying the adsorption of small molecules on the *platinum group of metals* is inadequate in capturing the complete catalytic activity of the magnetically polarized transition metal (TM) surfaces and proposed its generalization by invoking two distinct band centres for spin majority and spin minority d-electrons. We also demonstrated the potency of this extended d band model, by comparing the adsorption energies of NH_3 molecule on 3d-TMs obtained through spin-polarized density functional theory, with the ones which were predicted by our model [15].

First principles simulation of the oxide catalysts for SOFC applications

Our research colleagues (experimental) in Korea prepared lanthanide (Nd, Gd, Sm) doped BSCF and evaluated them in a way what they call “harsh SOFC operating conditions” such as Wind and Dry Cyclic Mode operation. The finding was *lanthanum doping increases the stability of the cathode for long term operations* and performance-wise Nd doping produces the best result. We explained their findings in terms of p-band centre of doped BSCF. We found that the doping of lanthanide shifts the p-band centre to low-

er energy, resulting in better stability and activity of these materials with respect to pure BSCF. For Nd doping this shift has an optimal value and therefore Nd doped BSCF shows the best performance [16].

Conclusion and outlook

Role of charge transfer, magnetism and strain in the heterogeneous catalysis are analysed. Especially in the context of alloy catalysts, combining these effects together in different ways can help in engineering efficient and cheap catalysts restricted not only for the fuel cell applications. The role of magnetism in the heterogeneous catalysis is not discussed extensively anywhere, and our formulation of spin dependent d band centre model is an extremely important step towards studying chemical reactions on metal surfaces with large spin polarization. One of the major advantages of such formulation is that one can now include the effect of magnetic field in the band energies of the catalysts to study how electrochemical kinetics can be altered through the magnetic field. Prior to that, the role of the magnetic field in heterogeneous catalysis used to be described in terms of the force exerted on the paramagnetic reactant molecules by the applied magnetic field.

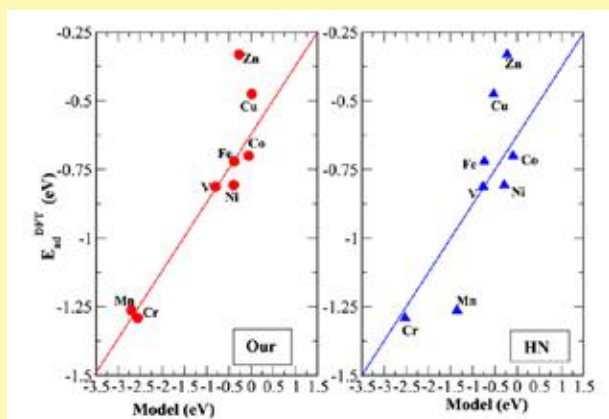


Figure 2 Comparison of the results of the proposed d-band center model (Our) with the standard d-band center model (HN). This work was published in Scientific Reports, 6, 35916 (2016)

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CINEMAS – New Integrated Platform for Materials Simulation



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Introduction

High-throughput computations have provided new pathway for advanced materials engineering and modelling. This has been possible by advent of rapidly growing capabilities of high performance computations and newly designed materials databases like “materials-project” or “Nomad”. Calculations which so far have been seen and interpreted as an individual data set only, can now be collected together in order to construct a database. By making an intelligent use of these techniques, simulations database can be used to predict trend/behavior in the existing data points or scan whole system to find new potential candidates for desired property/behavior.

Automation and management of huge number of calculations and resultant data requires a software (SW) platform to execute this task. Such a SW platform should take care of several stages of executing a single calculation, post-submission tasks like data analysis and a user-friendly customization of output graphical data for publication purpose. This SW platform, currently being developed at

IKST, is christened **CINEMAS**, an acronym for Comprehensively **I**ntegrated **E**nvironment for advanced **M**aterials **S**imulations.

Objective

The main objective of CINEMAS is to facilitate a large number of collective calculations for materials simulations. Such facilitation will include both single simulation (job) submissions as well as towards curating a database. Design of the interface shall be intuitive enough for even non-theorist to perform basic simulations. From each such simulations performed, CINEMAS shall retrieve, sort and store data to create a materials database for advanced material design and modelling. Fig. 1 indicates flow of each job that includes preparation of input files, connecting to the remote server, sending input files to server, execute the quantum engine on the files, retrieve the data back to local machine, analyze the data, sort the data and store it on the database.

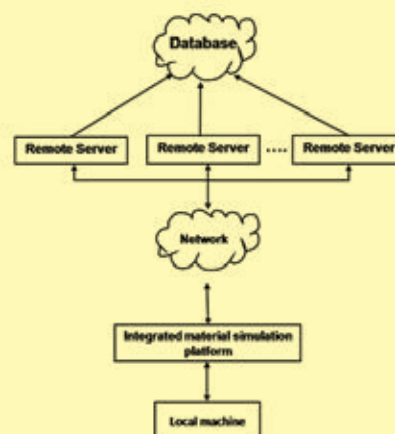


Figure 1 Execution of a job and storing data to database

Structure of CINEMAS GUI

CINEMAS is being developed on a plug-in based architecture with a central module CASCADE as its backbone. This module is a playground for work-flow of several simulation jobs to be executed. To start with, CINEMAS shall have an interface with atomistic DFT quantum engines only. Even within the purview of atomistic (DFT) calculations CINEMAS shall be flexible to switch between different quantum engines. More quantum engines

of higher length scale shall be developed and integrated to CASCADE as plug-ins in the future. It is also planned to integrate several external higher length scale codes seamlessly to CINEMAS. CINEMAS shall also provide GUI integration for externally developed quantum engines and auxiliary post-processing scripts as well.

CINEMAS has five major components which are briefly explained below:

1. CINEMAS–Cascade

CINEMAS–cascade is a central module to manage, execute, and monitor simulations (jobs) as well as exchange data between local machine and remote servers and finally analyze the output, as shown in Fig. 2. And all other modules are integrated to CASCADE as plug-ins. CINEMAS–cascade has the interdependency, parent-child, conditional statements type relationships among all the jobs. Seamless data transfer between different jobs can easily be performed.



Figure 2 CASCADE

2. CINEMAS–View

CINEMAS–View is state-of-the-art viewer module connected to CASCADE. At any point while working over any job from CASCADE, user can call this component to visualize atomic structure related to that job (Fig. 3). This can perform all modern tasks like volumetric data plotting / lattice-plane chopping / polyhedral creations etc. User has full freedom to choose and manipulate everything, unlike many other platforms, where these actions can be performed only in a pre-formatted manner. CINEMAS–View also provides very advanced “structure manager” to manipulate bulk structure of any geometry to create sur-

faces, finding adsorption sites on a surface, Nano-geometries, twin-boundaries and etc.

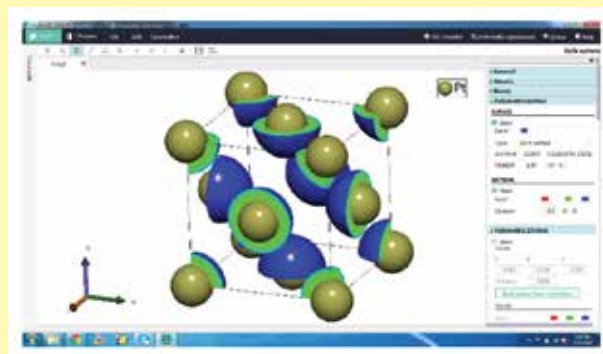


Figure 3 CINEMAS–View

3. CINEMAS–Plot

CINEMAS–Plot is a 2D-data plotter seamlessly connected with CASCADE and VIEW through a very friendly UI. CINEMAS–Plot also has an automatic interface with CASCADE to filter out different single value parameters as well as tabulate data from output files and plot them (Fig. 4). It has also the ability to perform advanced machine learning regression operations as well.

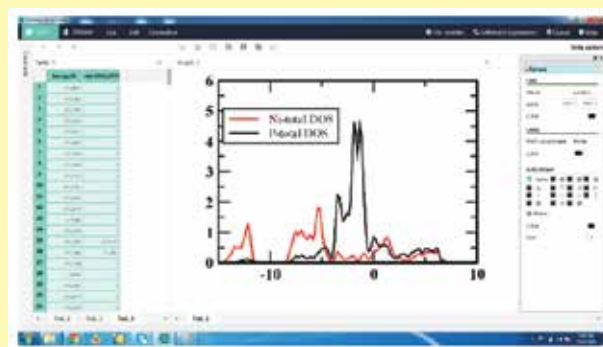


Figure 4 CINEMAS–Plot

4. CINEMAS–Draw

CINEMAS also provides an in-built drawing application to import graphics from CINEMAS–View and CINEMAS–Plot, manipulate and prepare publication quality figures, which are ready to put into a manuscript. This will have all drawing features with scientific inputs to assist preparation of figures.

5. CINEMAS–Auxiliary

a. Arithmetic module: CINEMAS has a module to perform arithmetic on the output from a job or a collection of jobs. There is a tailored arithmetic module interface within CINEMAS,

where arithmetic formulae can be defined using several keys from the same jobs or multiple ones. This formula can be defined and performed before or after execution of jobs. Depending upon finishing state of the job and output files result of such a formula will be displayed. Depending upon user's choice, same formula and corresponding results can be saved and exported to a ".csv" file for further analysis.

b. Pre-defined calculations module: CINEMAS has several calculations module which are already defined. These modules are like empty templates which contains several sequential/parallel job flows. User has to define systems and other instruction parameters, and jobs can directly be submitted on compute servers. CINEMAS has many such modules viz. DOS, BAND, NEB, Berry-phase, Phonons, polarization, etc.

Salient features of CINEMAS

1. CINEMAS considerably reduces number of steps to execute the simulations as compared to when it is done from command line, as well as other available simulation platforms.
2. Immaterial of Quantum computing engine chosen by user (VASP or ESPRESSO or SIESTA), front end GUI remains same throughout.
3. CINEMAS GUI takes all the inputs in general language. Thus, it allows even a non-theorist user to perform calculations with a minimal knowledge of a particular quantum engine. Based on the quantum engine is chosen, CINEMAS itself interprets the input instructions and prepares files accordingly.
4. CINEMAS has a seamless module that allows connectivity and file transfer between local machine and remote server(s).
5. As all the file-transfers take place in the back-ground, CINEMAS GUI is fully usable even when file transfers are going on between local machines and compute servers.
6. As CINEMAS provide a platform to perform

sequential actions – preparing input files, submission, processing, plotting, etc. lot of time is saved to execute simulations.

Future Outlook

In future CINEMAS shall emerge as a very comprehensive simulation platform, versatile enough to carry out pieces of small tasks as well as execute a large number of collective simulations. Construction of these databases shall also facilitate designing and developing machine learning algorithms for advanced materials design and modelling. Integration of higher-length quantum engines to CINEMAS is also part of the future plans. Thus, CINEMAS shall have great advantage over other existing simulation platforms.

Development of algorithms for computer vision and pattern recognition



Renuka Patnaik
Research Associate
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Introduction

Software employing computer vision algorithms have become ubiquitous, finding applications in biometric authentication, facial feature tracking, video surveillance, robotics etc. In the context of video analytics, one of the objective is to process large number of videos, with minimal human supervision or intervention. Such autonomous video-processing methods can be used for motion detection, abnormal event detection, object detection and recognition and license plate reading, creating a video synopsis, people counting, traffic monitoring, etc. IKST, in collaboration with academic institutes, has developed such software applications which are currently in use by KIST researchers. Brief summary of this work is presented below.

IKST also works in the area of data analytics for medical informatics by building machine learning models based on the person specific data and predicting the likelihood of occurrence of a particular disease.

Work in IKST

Machine learning library: A C library was developed for Regression using Machine

Learning (ReML). The library includes ridge regression, LASSO [3], kernel ridge regression [4], support vector machine [2], Bayesian regression and Bayesian ridge regression. This library will be useful for big data applications like material informatics, health informatics, etc. The library was tested on the data, generated in IKST lab for predicting the energy of materials. The results are in par with those obtained from python library as shown in Fig. 1. To validate ReML library further, we are using electronic health records to correlate health of an individual to various parameters, both extrinsic and intrinsic.

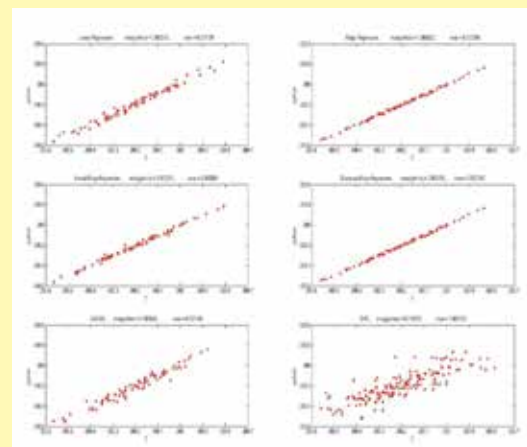


Figure 1 Comparison of results for various methods with python library

Collaborative Work

a. PES University

1. *L1 magic library in C:* L1-MAGIC is a collection of MATLAB routines for solving the convex optimization programs central to compressive sampling. Compressive sensing is a theory of signal recovery from highly incomplete information; data can be recovered from a small number of linear measurements by solving a convex program. L1-Magic package [9] implements this recovery procedure in seven contexts. The algorithms are based on standard interior-point methods, and are suitable for large-scale problems. The main aim of this project is to port L1-magic problems from MATLAB functions to C using OpenCV libraries and some of the common libraries, built particularly to execute the project. The code uses GPU to reduce the running time. This project is collaborative work with Dr. V. K. Agarwal, Professor, Department of Information Sci-

ence, PESIT, Bengaluru.

For validation of this library, a face recognition module was developed in-house for classification [1][2] of facial images. The recognition rate is computed for a desired combination of feature, classifier and dimension, represented by $C = (f \in F, d \in D, cl \in CL)$. The set of features is given by $F = \{\text{Eigen, Fisher, random and down-sample}\}$. The set of classifiers is given by $CL = \{\text{SRC, SVM, NN, NS}\}$, where SRC is sparse representation classifier [5], SVM is support vector machine, NN is nearest-neighbor and NS is nearest sub-space. The set of dimensions is given by $D = \{30, 56, 120, 504\}$. The plots of recognition rates for different combinations is shown in Fig. 2.

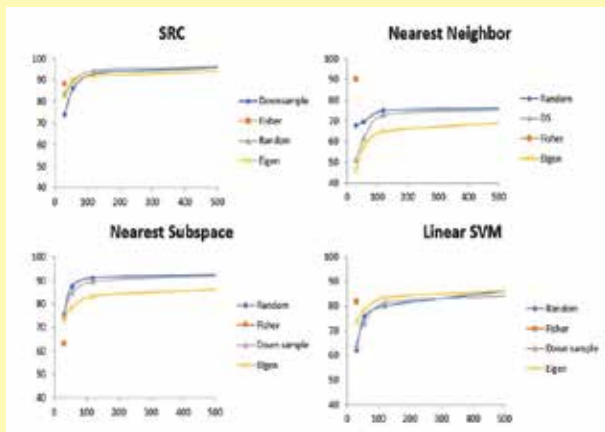


Figure 2 Recognition rates for different combinations, $C = (f, d, cl)$

2. Supervised descent method for face alignment: The objective of this project is to develop robust, efficient and computationally inexpensive technique for identifying facial landmarks. Supervised Descent Method [6] was implemented for this purpose. This method learns a sequence of descent directions iteratively during the training session. The parameters learnt in the training session are subsequently used in the testing phase. In the testing phase, the learnt descent directions are used to converge the initial configuration of the facial landmarks to the actual landmarks without undergoing complex calculations (see Fig. 3). This project is collaborative work with Dr. Shylaja, Head of the Department of Information Science, PESIT, Bengaluru.

b. IIT Bhubaneswar

1. Abnormal Event Detection: Speedy abnormal event detection meets the growing de-

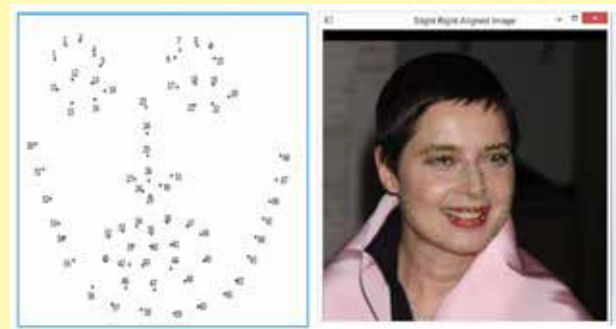


Figure 3 Initial configuration of landmarks (left) and after alignment (right)

mand to process an enormous number of surveillance videos. Based on inherent redundancy of video structures, this project implements efficient sparse combination learning framework [7], based on 3D gradient features, computed on each spatio-temporal cubes of all frames. This approach directly learns sparse combinations, which increase the testing speed hundreds of times. The authors of the original work have provided the MATLAB implementation source code of the algorithm and the same has been implemented using OpenCV C++ development environment along with GUI. This can be used for real-time detection of abnormal events and thus can be used for the prevention of untoward incidents without any delay by taking proper action by the authorities using the surveillance system.

2. Motif Analyzer: This project focuses on mining recurrent temporal patterns [8] (motifs), in multivariate time series with as little supervision as possible. This elementary task can be useful for applications like summarizing a scene, counting or detecting particular events, or detecting unusual activities. More generally, this identification of temporal motifs and the instant at which they occur can be used as a dimensionality reduction method for (potentially supervised) higher level analysis. One major challenge comes from the fact that time series that we observe are often “caused” by a superposition of different phenomena recurring in time and with no specific synchronization. In the context of video sequences, the specific goal is to find activity patterns (e.g., car passing, pedestrian crossing) without supervision. The scope of this project is to implement Motif analyzer [8]

based on the traffic video from a static camera in OpenCV platform. In the first phase, a video captured from a static camera is converted into a temporal document using PLSA algorithm. In the second phase, the temporal document is used to identify the motif and its occurrence time using Dirichlet Process. The motif obtained from a publicly available dataset, *virat* is shown in Fig 4.

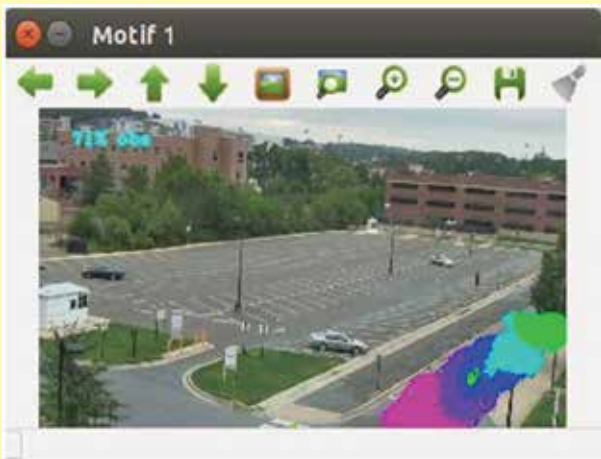


Figure 4 Result of motif analyzer

3. *Video Synopsis*: Video synopsis [10] is an effective tool for browsing and indexing of videos from surveillance cameras that operate 24 hours/day. It provides a short video representation, while preserving the essential activities of the original video, which otherwise is a time-consuming procedure. This process includes two major phases: i. an online conversion of the endless video stream into a database of objects and activities (rather than frames) and ii. a response phase, generating the video synopsis as a response to the user's query. The primary objective of the project (on-going) is to implement the video synopsis algorithm and analyze / optimize the implementation of the algorithm using C/C++ framework with adequate GUI support.

Projects, 3.b.i, 3.b.ii and 3.b.iii were carried out in collaboration with Dr. Debi Prasad Dogra, Assistant Professor, School of Electrical Sciences, IIT Bhuvanewar.

Outlook

There is possibility to expand the work on predictive analysis, based on individual

data using electronic health records obtained at different time stamps to analyze his/her health progress and video synopsis, which are on-going projects.

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Summary of Collaborative Research Projects – Physical Sciences



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IKST currently has active collaboration with two research institutes: *Jawaharlal Nehru Centre for Advanced Scientific Research* (JNCASR) and *Indian Institute of Science* (IISc.) both situated in Bangalore.

IKST is collaborating with Prof. U. V. Waghmare, Prof. Shobhana Narasimhan and Prof. Swapan Pati of JNCASR. With Prof. Waghmare our collaboration is in the field of electro-catalysis and the study of nature of bonding in the solids. Prof. Waghmare's group is involved in the development of a descriptor to analyse the chemical bonding in the solids known as Distribution of Electron Charge Centres (DECC).

Prof. Shobhana Narasimhan is collaborating in a project to identify cheap, efficient catalysts for important chemical reactions such as reduction of NO_x gases in automobile exhaust using first-principles based methods.

Prof. Swapan Pati is involved with IKST in the field of study of transport properties of two-dimensional semiconductors using Boltzmann transport formalism within acoustic deformation potential approximation.

Prof. Manish Jain, department of Physics, IISc, through collaboration with

IKST has already developed a nudged elastic band module (a computational tool useful for studying the transition state of a chemical reaction), which can be interfaced with density functional theory based simulation codes such as SIESTA, Quantum Espresso and VASP. Presently Prof. Jain's group and IKST are working together to develop certain post processing tools which will be used to analyse chemical bonding, magnetic exchange interactions in solids etc.

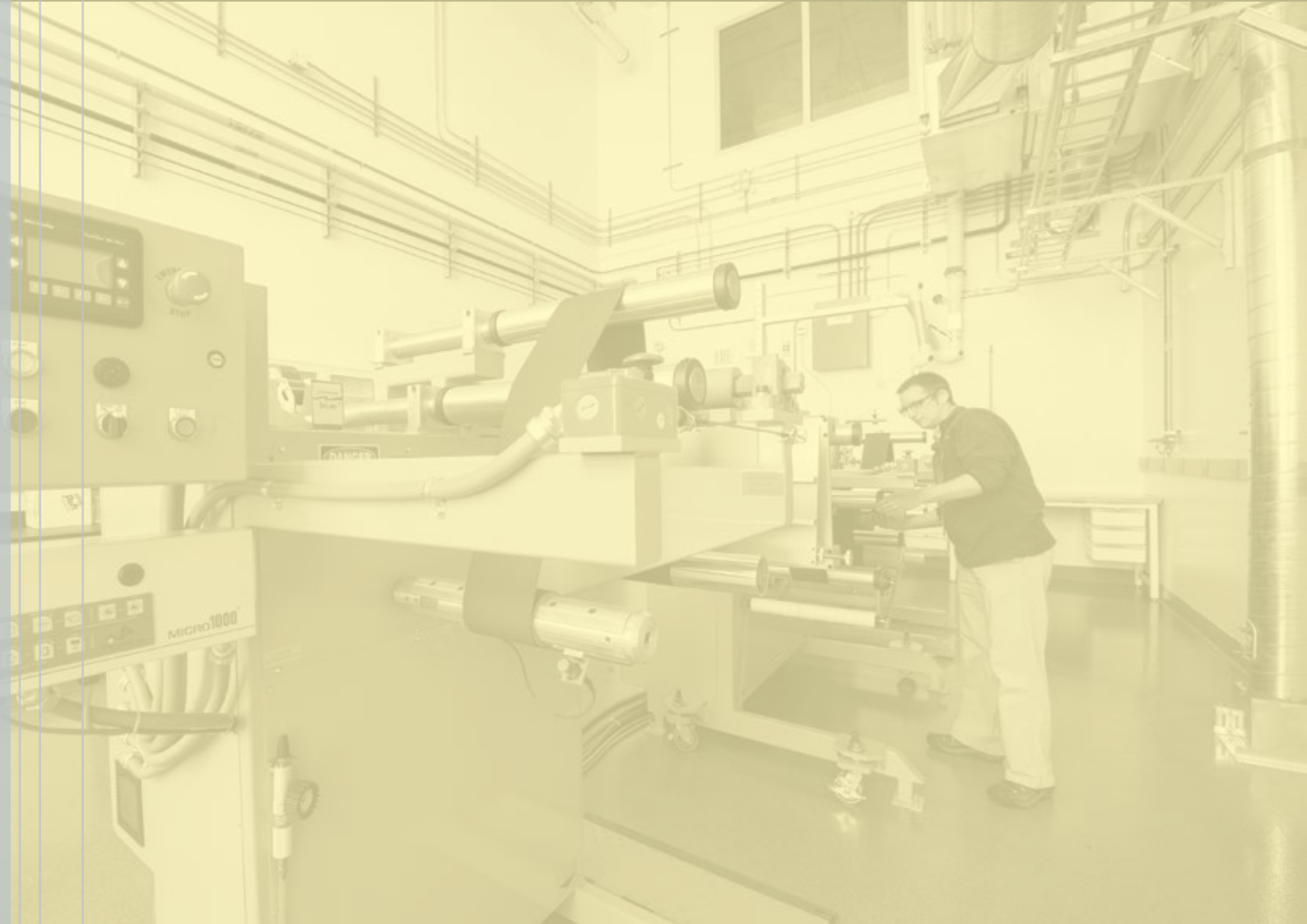
List of Publications

2015

Sl. No.	Author(s)	Title	Journal
1	Jungho Shin, Jung-Hae Choi, Pil-Ryung Cha, Seong Keun Kim, Inho Kim, Seung-Cheol Lee, Doo Seok Jeong	Catalytic activity for oxygen reduction reaction on platinum-based core-shell nanoparticles: all-electron density functional theory	<i>Nanoscale</i> Vol. 7, October 2015 pp. 15830–39
2	Jongseob Kim, Seung-Cheol Lee, Sung-Hoon Lee, Ki Ha Hong	Importance of Orbital Interactions in Determining Electronic Band Structures of Organo-Lead Iodide	<i>The Journal of Physical Chemistry C</i> Vol. 119, March 2015 pp. 4627–34
3	Seok Ki Kim, Dohyeon Yoon, Seung-Cheol Lee, Jaehoon Kim	Mo ₂ C/Graphene Nanocomposite as a Hydrodeoxygenation Catalyst for the Production of Diesel Range Hydrocarbons	<i>ACS Catalysis</i> Vol. 5, June 2015 pp. 3292–303
4	Satadeep Bhattacharjee, Kapil Gupta, N. Jung, S. J. Yoo, Umesh V. Waghmare, S. C. Lee	Site preference of NH ₃ -adsorption on Co, Pt and CoPt surfaces: the role of charge transfer, magnetism and strain	<i>Physical Chemistry Chemical Physics (PCCP)</i> Vol. 17, April 2015 pp. 9335–40
5	Na-Young Park, Ho-Seok Nam, Pil-Ryung Cha, Seung-Cheol Lee	Size-dependent transition of the deformation behavior of Au nanowires	<i>Nano Research</i> Vol. 8, March 2015 pp. 941–47

2016

Sl. No.	Author(s)	Title	Journal
1	Satadeep Bhattacharjee, U. V. Waghmare, S. C. Lee	An improved d-band model of the catalytic activity of magnetic transition metal surfaces	<i>Scientific Reports</i> Vol. 6, November 2016 pp. 35916-1-10
2	Tae-Hee Lee, Ka-Young Park, Nam-In Kim, Sun-Ju Song, Ki-Ha Hong, Docheon Ahn, Abul Azad, Junyeon Hwang, S. Bhattacharjee, Seung-Cheol Lee, Hyung-Tae Lim, Jun-Young Park	Robust $\text{NdBa}_{0.5}\text{Sr}_{0.5}\text{Co}_{1.5}\text{Fe}_{0.5}\text{O}_5$ cathode material and its degradation prevention operating logic for intermediate temperaturesolid oxide fuel cells	<i>Journal of Power Sources</i> Vol. 331, November 2016 pp. 495-506
3	Ko Y. J., Cho J. M., Kim I., Jeong D. S., Lee K. S., Park J. K., Baik Y. J., Choi H. J., Lee S. C., Lee W. S.	Inherently-forced tensile strain in nanodiamond-derived onion-like carbon: Consequences in defect-induced electrochemical activation	<i>Scientific Reports</i> Vol. 6, April 2016 pp. 23913-1-10
4	Satadeep Bhattacharjee, S. J. Yoo, Umesh Waghmare, S. C. Lee	NH_3 adsorption on PtM (Fe, Co, Ni) surfaces: Cooperating effects of charge transfer, magnetic ordering and lattice strain	<i>Chemical Physics Letters</i> Vol. 648, March 2016 pp. 166-169
5	Namgee Jung, Satadeep Bhattacharjee, Sanjeev Gautam, Hee-Young Park, Jaeyune Ryu, Young-Hoon Chung, Sang-Young Lee, Injoon Jang, Jong Hyun Jang, Sae Hum Park, Dong Young Chung, Yung-Eun Sung, Keun-Hwa Chae, Umesh V. Waghmare, Seung-Cheol Lee, Sung Jong Yoo	Organic-inorganic hybrid PtCo nanoparticle with high electrocatalytic activity and durability for oxygen reduction	<i>NPG Asia Materials</i> Vol. 8, January 2016 pp. 237-1-10
6	Young-Hoon Chung, Kapil Gupta, Jue-Hyuk Jang, Hyun S. Park, Injoon Jang, Jong Hyun Jang, Youg-Kul Lee, Seung-Cheol Lee, Sung Jong Yoo	Rationalization of electrocatalysis of nickel phosphide nanowires for efficient hydrogen production	<i>Nano Energy</i> Vol. 26, August 2016 pp. 496-503



Activities

Workshops & Seminars

2015

*JNCASR-IKST-UCL Winter School on
Materials and Processes for Application
in Energy and Environment*

Dates

January 15–18

Venue

JNCASR, Bengaluru

Conveners

Prof. Richard Catlow (UCL)

Dr. Seung-Cheol Lee (IKST)

Prof. Umesh Waghmare (JNCASR)

Objectives

Knowledge Dissemination Topics:
Modeling and prediction of structure and
materials, Thermo-electrics, catalysis,
solar water splitting, photovoltaics,
fuel cells, gas and energy storage,
Electrochemistry, Advanced computational
techniques (Meta-dynamics & GW)

Participants

15 lecturers, 7 IISc. Faculty, 18 JNCASR
Researchers, 7 participants from the
Industry, 26 outstation participants,
5 participants from Bangalore



*IKST-JNCASR Joint Workshop on
Promotion of Collaborative Research*

Date

July 21

Venue

JNCASR, Bengaluru

Conveners

IKST

JNCASR

Objectives

- i. To build Indo-Korea relationship as Global Knowledge Platform (GKP) project in S&T area.
- ii. To draw out joint research projects in areas of computational science, theory and data analysis.

Participants

Dr. Seung-Cheol Lee

Dr. Satadeep Bhattacharjee

Dr. Kapil Gupta

Ms. Renuka Patnaik

Dr. Mahesh Chandran

(IKST)

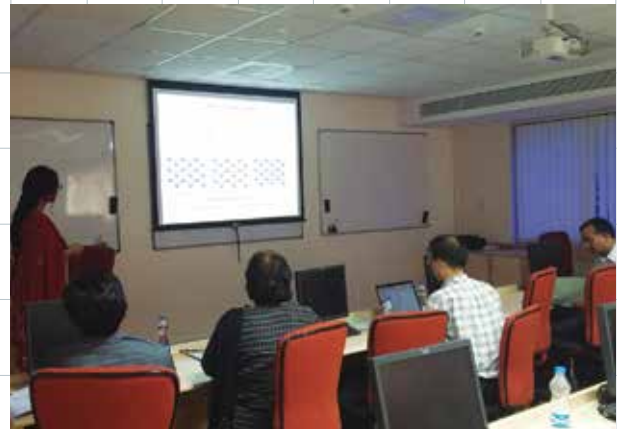
Prof. Umesh Waghmare

Prof. Balasubramanian Sundaram

Prof. Shobhana Narasimhan

Prof. Swapan Pati

(JNCASR)



KIST-IKST-JNCASR Joint Workshop on Innovative Materials

Dates

November 30 to December 1

Venue

KIST, Seoul

Conveners

KIST

IKST

JNCASR

Objectives

- i. To enhance Indo-Korea R&D cooperation.
- ii. To explore and develop joint research projects in the areas of material design, next generation devices, computational materials science and structural materials.

Participants

Dr. Doo Seok Jeong

Dr. Jae Hyuk Shim

Dr. Jung Hae Choi

Dr. Jin Dong Song

Dr. Sang Soo Han

Dr. Seungchul Kim

Dr. Woo Sang Jung

Dr. Sung Jong Yoo

(KIST)

Dr. Seung-Cheol Lee

Dr. Satadeep Bhattacharjee

Dr. Kapil Gupta

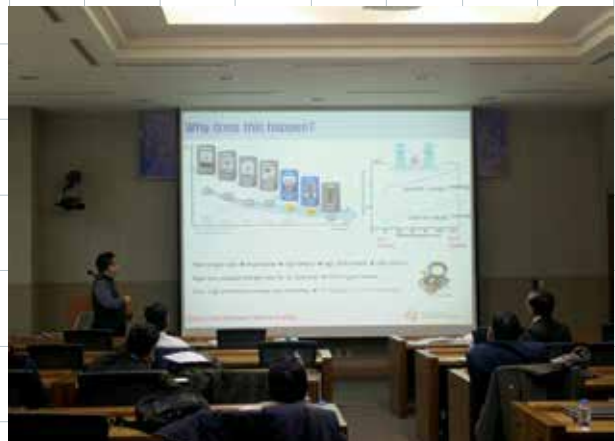
Dr. Mahesh Chandran

(IKST)

Prof. Umesh Waghmare

Prof. Swapan Pati

(JNCASR)



*IKST-IISc Joint Workshop on
Advanced Materials and Modelling*

Date

December 21

Venue

Movenpick Hotel, Bengaluru

Conveners

IKST

IISc.

Objectives

To explore and develop joint research
projects for 2016

Participants

Dr. Seung-Cheol Lee

Dr. Satadeep Bhattacharjee

Dr. Kapil Gupta

Dr. Mahesh Chandran

(IKST)

Prof. Vikram Jayaram

Prof. T A Abinandanan

Prof. Abhishek Singh

Prof. Abhik N. Choudhury

Prof. S Kathikeyan

Prof. Praveen Kumar

Prof. Ramsharan Rangarajan

(IISc.)



2016

IKST-CU Joint Seminar on Computational Science: An Innovation Tool for R&D in Science and Technology

Dates

September 6–7

Venue

Christ University, Bengaluru

Conveners

IKST

Centre for Digital Innovation, CU

Objectives

- i. To build Indo-Korea R&D Network by connecting government and private R&D organizations.
- ii. To promote mutual understanding in IT area between India and Korea by sharing information.
- iii. To facilitate possible cooperation among participants through one to one meetings.

Participants

INDIA:

Dr. Seung-Cheol Lee

Dr. Ravikumar M V

Dr. Satadeep Bhattacharjee

Dr. Kapil Gupta

Dr. Mahesh Chandran

(IKST)

Dr. Anil Joseph Pinto (CU)

Dr. A V N Krishna (CU)

Mr. Shinto Joseph (LDRA Technology)

Dr. Anil Kumar A R (Fluidyn Consultancy)

Dr. Sitaram Naik (Embitel)

Mr. Ashwin Thondavadi (Bosch Engineering)

Prof. Debi Prosad Dogra (IIT BBS)

KOREA:

Dr. Jeong Tae Kim (KITECH)

Kyungwon Tech (KITECH)

Dr. Sung Sik Shin (KITECH)

Mr. Kwang Won Seo (S&WISE)

Dr. Sung Yoon Lee (S&WISE)

Dr. Seungchul Kim (KIST)

Mr. Chan Soo Kim (KIST)



IKST Internal Workshop

Date

December 16

Venue

Taj KIA, Devanahalli

Objectives

- i. To review the performance of 2016.
- ii. To share the plan for 2017.

Participants

Management and Staff of IKST

Mrs. Lee, Dept. of International Cooperation,
KIST



Special Lectures delivered by IKST Researchers in 2016

*“Role of S&T in Korea’s Economic
Development: Case of KIST”*

April 1

Indian Institute of Science, Bengaluru

Resource Person

Dr. Seung-Cheol Lee

Summary

This lecture was delivered to Post-graduate Technology Management Students of Dept. of Management Studies, IISc. The lecture highlighted how after the end of Korean war, since the foundation of KIST in 1966, the size of Korea’s economy developed by a thousand times. It highlighted the important role played by KIST in building strategy and developing technologies. The presentation also showcased how during the next fifty years KIST will focus on bridging fundamental science and innovative industry.



“How to Develop SW in India”

May 31

KITECH, Seoul

Resource Person

Dr. Seung-Cheol Lee

Summary

This lecture was delivered to researchers of KITECH.

- i. Shared experience on SW development in India.
- ii. Differences between development of SW in India and in Korea.
- iii. Invited them to the IKST-CU Joint Seminar.



“Current Research Activities of IKST and Design of Alloy and Compound Catalysts for Fuel Cell Applications”

September 24
SRM University, Chennai

Resource Person
Dr. Seung-Cheol Lee

Summary
Invited lecture

~

“Current Research Activities of IKST in the area of Computer Vision”

October 22
Indian Institute of Technology, Bhuvaneshwar

Resource Person
Ms. Renuka Patnaik

Summary
In the audience were graduate students of IIT-BBS who participated in the IEEE Students Colloquium 2016, hosted by IIT BBS. The objective of the talk was to strengthen the collaboration between IIT BBS and IKST in the areas of computational geometry, video analytics and machine learning through collaborative research and exchange programs.



“Multicomponent Descriptor based Analysis of Catalytic Activity of Bimetallic Alloy”

November 8
ENGE 2016, Seoul

Resource Person
Dr. Seung-Cheol Lee

Summary
Invited lecture

~

“Role of S&T in Korea’s Economic Development: Case of KIST”

December 21
Christ University, Bengaluru

Resource Person
Dr. Seung-Cheol Lee

Summary
The audience comprised delegates who participated in the 9th KSTA S&T Conference. Presentation highlighted brief historical background of Korea after Korean Civil War. The war destroyed all the infrastructure and human resources. Since the foundation of KIST in 1966, Korea’s economy became a thousand times bigger. KIST had played an important role for building strategy and developing technologies. The next 50 years of KIST will focus on bridging fundamental science and innovative industry.



Memorandum of Understanding with *Karnataka Science and Technology Academy (KSTA)*

KSTA was initiated in July 2005 by the *Department of Science & Technology (DST)*, Government of Karnataka in order to promote S&T related activities in the state as well as to popularize science among civil society, especially the rural areas. KSTA has been playing a pivotal role in popularizing science education among rural schools through several programs – KSTA Fellowship, Annual Conference in which national-level and international-level scientists speak on current S&T topics, special lecture series, training trainers, and awards for science writers in local language, among others.

In December 2015 IKST signed a MOU with KSTA to facilitate an Exchange Program between Karnataka State and Korea, as well as to conduct Technology Forums / Workshops / Seminars on chosen topics of mutual interest. While **Dr. Seung-Cheol Lee**, Director signed the MOU on behalf of IKST, **Dr. Honne Gowda**, Secretary, KSTA and Managing Director, *Karnataka Science & Technology Promotion Society (KSTEPS)* signed on behalf of the Government of Karnataka.



Memorandum of Understanding with *Christ University (CU)*

IKST signed a revised MOU with CU in October 2016 to promote Industry–Research initiatives in Software through specialized seminars / forum to develop a platform for Small and Medium Enterprises from Korea to interact with their counterparts in India mainly in the ICT sector. The MOU was signed by **Dr. Seung-Cheol Lee**, Director on behalf of IKST and **Dr. Anil Joseph Pinto**, Registrar signed on behalf of CU.



Visitors to IKST 2015

Dr. Tae Hoon Lim

Vice President, KIST

August 25

Places visited

IKST, JNCASR and KSTA

Brief summary

- ▷ Dr. Tae-Hoon Lim formally inaugurated the new IKST office at *NCC Urban Windsor*. Dr. Seung-Cheol Lee presented the current status of IKST and future plans.
- ▷ Dr. Lim called on Prof. C. N. R. Rao, Chairman, ICMS and former President, *JNCASR*.
- ▷ Dr. Lim called on Dr. Honne Gowda, MD, *KSTEPS*, Government of Karnataka.



Dr. Dong Hwa Kum

Fellow, KIST

Former President, KIST

October 18–23

Places visited

IKST, JNCASR and IISc.

Brief summary

- ▷ Dr. Seung-Cheol Lee presented the current status of IKST.
- ▷ Dr. Kum visited Divisional Chairman, Mechanical Sciences, *IISc.* and discussed possible R&D cooperation and collaboration.



2016

Dr. In Hwan Oh

Director General, Green Technology Institute, KIST

November 5

Places visited

KSTA and IKST

Brief summary

▷ Dr. Oh participated KSTA 8th Annual Conference at Bangalore Institute of Technology and delivered a lecture titled “Green Technologies for Gen-Next City”



Ji Hwan Shin

Sunchon National University

January 8 to February 3

Places visited

IKST

Brief summary

▷ Performed collaborative research on “Prediction of Mechanical properties of alloys by using first principles calculation”



Visitors to IKST 2016

Dr. Eui-Jin Jun

Principle Auditor & Director, KIST

January 18-22

Places visited

IKST, JNCASR and IISc.

Brief summary

- ▷ Dr. Seung-Cheol Lee reported the current operation of IKST.
- ▷ Discussion on measures of systematic and efficient operation of IKST.
- ▷ Dr. Jun also called on the president of JNCASR and the divisional chairman of Mechanical Sciences, IISc.



Dr. Byeong-Gwon Lee

President, KIST

May 3

Places visited

IKST

Brief summary

- ▷ Dr. Seung-Cheol Lee presented the current status of IKST.
- ▷ Discussion on measures of strengthening Indo-Korea network.



Dr. Won-Kook Choi

Director of Materials and Life Science Research
Division, KIST

July 5

Places visited

IKST

Brief summary

▷ Discussion on cooperative research
between the Computational Science
Research Center of KIST and India.



Dr. Sang-Cheon Lee

Chairman, NST

July 6

Places visited

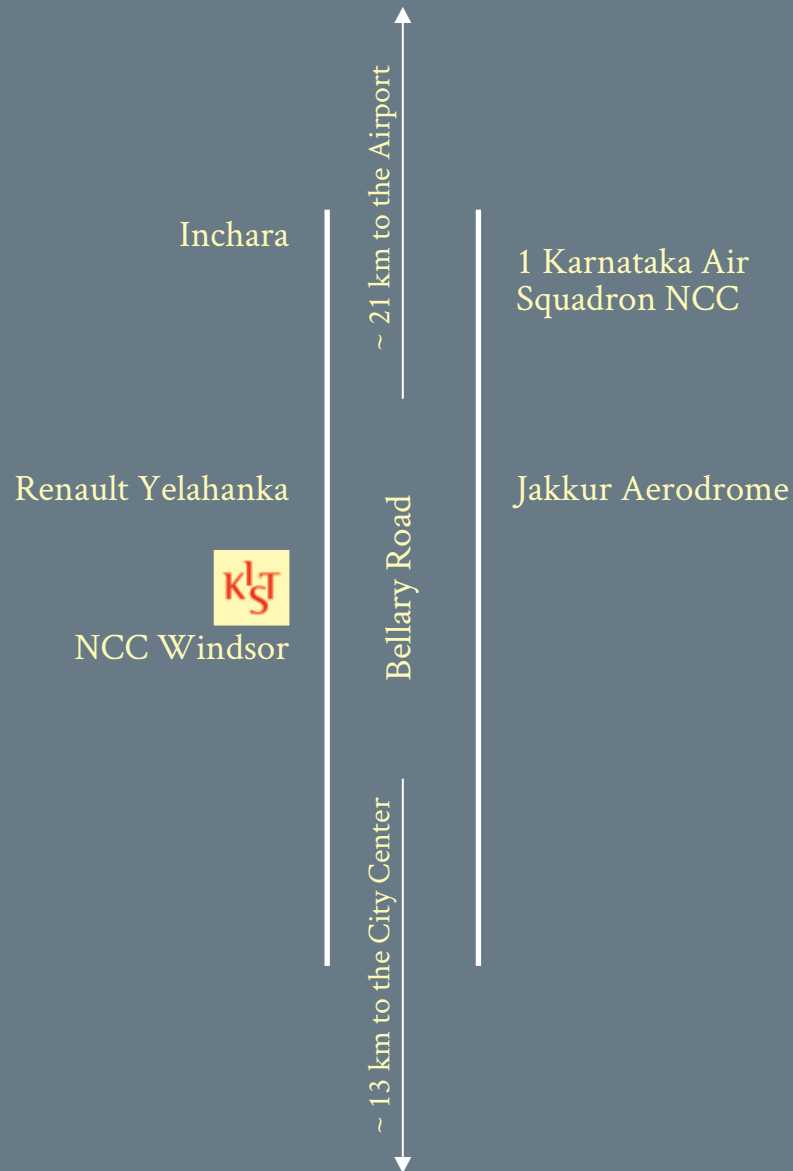
IKST

Brief summary

▷ Dr. Seung-Cheol Lee reported the current
status of IKST and measures of promoting
cooperation between Indian and Korea
Government R&D Institutes through IKST.







Indo-Korea Science and Technology Center (IKST) is a **Section 8** company as per **Indian Companies Act, 2013** (earlier Section 25 company as per Indian Companies Act, 1956).

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