AKSHAY SUBRAMANIAN

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EDUCATION

Indian Institute of Technology Roorkee   *August 2017 - August 2021*
In Progress
Bachelor in Technology (B.Tech.)
Metallurgical and Materials Engineering   Cumulative GPA: **9.309**/10

National Public School, Bangalore, India   *June 2016 - May 2017*
Computer Science Stream
Central Board of Secondary Education (CBSE)   Overall Percentage: **96.0**

RESEARCH EXPERIENCE

Extraction of insights from Gold nanoparticle synthesis literature using Computer Vision and NLP techniques
Prof. Gerbrand Ceder | Lawrence Berkeley National Laboratory (LBNL), Berkeley

- Working on identifying interesting correlations between **synthesis recipes** and **synthesis outcomes** in **gold nanoparticle** synthesis by mining text and images from Materials Science literature. **Machine Learning** techniques are being used for information retrieval from papers and subsequent analysis.

- Part of the team developing [**CovidScholar**]. The aim of this effort is to curate and tag **COVID-19 related research work** to make them easily accessible to researchers and thereby accelerate research in this area. Relations between papers and tagging of papers into categories are achieved using **NLP** and **Machine Learning** based approaches. **A paper based on this work is under preparation**.

Inverse Design of Potential Singlet Fission Molecules using a Transfer Learning Based Approach
Prof. Soumitra Satapathi | Indian Institute of Technology Roorkee
Implemented a **deep generative model** to predict potential **Singlet Fission** molecules for Solar Cell applications. To overcome the issue of data scarcity, we propose a **transfer learning** approach. A paper based on this work has been **submitted for publication** in a journal and is under review.
[**arxiv preprint**]

Multitask Learning to predict crystal strains from EBSD diffraction patterns
Prof. K.S. Suresh | Indian Institute of Technology Roorkee
Implemented a **Deep Convolutional Neural Network** and employed **Multitask learning** to predict **crystal strain** components from **Kikuchi Diffraction Patterns**.

PyTorch Implementation of 'Optimization of Molecules via Deep Reinforcement Learning'
Individual Work
Implemented and reproduced the results obtained in **'Optimization of Molecules via Deep Reinforcement Learning'** by Zhou et al. Made a couple of improvements to the original implementation to stabilize training:

- Utilized an additional **target Q-Network** to stabilize training as opposed to the single Q-Network used in the original TensorFlow implementation by the authors.

- Updated the target Q-Network periodically using **Polyak averaging**.

[**Code on GitHub**]

PyTorch Implementation of 'Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules'
Individual Work
Implemented and reproduced the results obtained in **'Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules'** by Gomez-Bombarelli et al.
[**Code on GitHub**]

Repurposing Commercially available drugs for inhibition of the coronavirus using Machine Learning Techniques
Prof. Soumitra Satapathi | Indian Institute of Technology Roorkee
Experimented with a variety of **Machine Learning** techniques to predict potential **inhibitors** of the **SARS coronavirus** protease molecule. Among others, made use of **Graph Neural Networks**, **Random Forests** and vanilla **Deep Neural Networks**.

Investigation of effect of electric current loading on the morphology of the crack in thin sheets of metals
Prof. Praveen Kumar | Indian Institute of Science, Bangalore
Worked on a project titled '**Investigation of effect of electric current loading on the morphology of the crack in thin sheets of metals**'. Primarily worked on healing **fatigue cracks** in metal sheets by application of **electric pulses**.
[**Certificate**]

OPEN SOURCE CONTRIBUTIONS

Chainer *January 2019 - September 2019*
ChainerX is a versatile ndarray implementation with special support of deep learning-specific operations. I worked on supporting many **fundamental operators** usually available for ndarray libraries (e.g. those provided by NumPy and SciPy) as well as special operators focusing **deep learning** applications (e.g. convolution, pooling, activation functions, etc.).
[**Report**] [**Contributions**]

DeepChem April 2020
The **DeepChem** project is an open source framework that provides tools for drug discovery, materials science, quantum chemistry, and biology. I have implemented the approaches described in **'Optimization of Molecules via Deep Reinforcement Learning'** by Zhou et al. and **'ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition'** by Jha et al. into **TorchChem**, which is a PyTorch version of the DeepChem framework.
[**GitHub link**]

TECHNICAL SKILLS

Programming Languages	Python, C++, Javascript
Frameworks	PyTorch, Tensorflow, Keras, React.js
Software & Tools	Git, Docker, SLURM, MongoDB
Equipment and Instruments	Instron Fatigue test, SEM, Electrical Discharge Wire Cutting (EDSWC)

NOTABLE ACHIEVEMENTS

I am ranked **1st out of 80** students in my department at IIT Roorkee based on overall academic performance.

Was **one out of 150** students selected all over the country for the **Google AI Summer School 2020**.

Selected for the prestigious **MITACS Globalink Research Internship 2020** program that funds Summer research internships at Canadian Universities.

Was awarded the **IIT Roorkee Heritage Excellence Award 2019** for outstanding academic, co-curricular and extra-curricular achievements.

Was among the **top 0.1 percent** in the country in the **Chemistry** Examination of the 12th Grade CBSE Board Examinations.(Scored 100/100)

Was ranked **17th** in the state of Karnataka in the State Level **National Talent Search Examination 2015** and was awarded a scholarship by the Department of State Educational Research and Training (DSERT) for being one out of 151 students from Karnataka to qualify the examination.

EXTRA-CURRICULARS

Member of **Data Science Group, SDSLabs** - a group in campus responsible for fostering a culture of Data Science by organizing **Machine Learning** and **Deep Learning** related competitions and Lectures.

Awarded the **K.V. Mittal Memorial Award** twice for securing the **1st** position in the Institute Open **tennis** tournament held in 2017 and 2019.

Secretary of the IIT Roorkee **tennis team** for the session 2019-2020.

Captained the IIT Roorkee Tennis team at the prestigious **Inter IIT Sports Meet** held in IIT Madras in 2017, IIT Guwahati in 2018 and IIT Kharagpur in 2019.

Captain of **Tennis** and **Table Tennis teams**, National Public School Koramangala, Bangalore