# Evaluation of D.D., Major Project Part -1

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Project Title:   Surface Binding Energy Prediction using Machine Learning Models.

Marks obtained for the report number 1 / 2 / 3 / 4   are:        0 / 1 / 2 / 3
**(Students, please circle the appropriate report number)**

Report 1: 09 Aug 2019
Report 2: 02 Sep 2019
Report 3: 18 Oct 2019
Report 4: 01 Nov 2019

**Reports submitted later than the deadline will not be accepted.**

Summary of work done:

Extracted a dataset of around 87k catalytic reactions and applied five machine learning models including Linear regressor, Support Vector Regressor and Gradient boosting regressor, K Nearest Neighbours and Neural Networks to predict the binding energy of C on 111 surface. Optimised the code to produce 0.69 R square test value and 0.9 R square on training data set.

Future plan:

Apply different machine learning models on the data and find the best among them. Reduce the root mean square error of test dataset upto 0.3. Different feature selection and extraction and finding the feature importance. Built a general model for 111 surface to predict binding energy of Carbon and Oxygen

Signature of supervisor with date