

# Uncertainty Benchmark (placeholder)

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## Abstract

Abstract here.

## Introduction

1. ML/DS + catalysis<sup>1</sup>
2. Why uncertainty?
  - (a) want confidence on DFT predictions themselves
  - (b) active routines
3. Very quick overview of the paper (Figure 1)

## Methods

1. Data

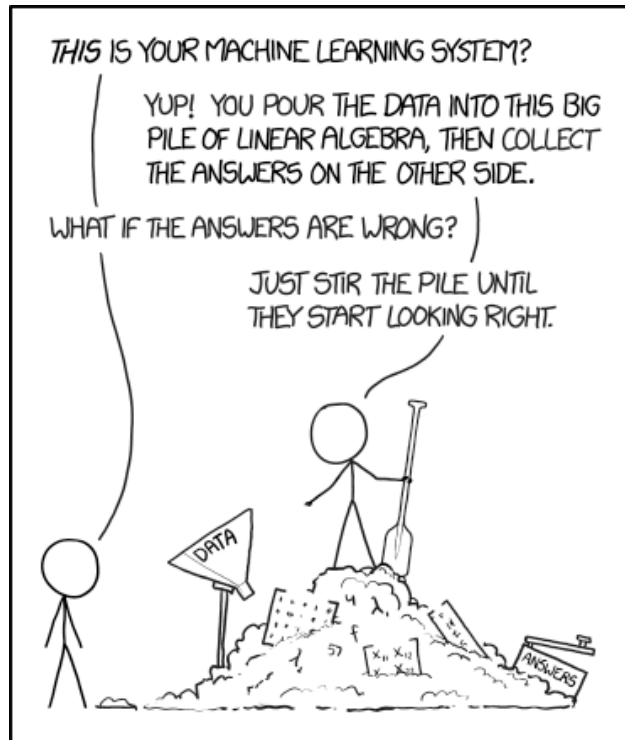


Figure 1: Placeholder for overview of the paper

- (a) GASdb
- (b) Splits
- (c) VASP(?)
- (d) Blocking (on best)

## 2. Modeling

- (a) CGCNN
- (b) CGCNN Ensemble
- (c) GP
- (d) GP with CGCNN
- (e) With other kernels too
- (f) Penultimate-Fed GP
- (g) Bayesian CGCNN with prior on weights at some layer

- (h) Supervised error prediction (delta CGCNN)
  - (i) Dropout CGCNN
3. Assessment
- (a) accuracy
  - (b) calibration
  - (c) sharpness

## Results

1. Table/figure of accuracies: MSE, MAE, R2, [willie get list]
2. Plots:
  - (a) Parity plots
  - (b) Calibration/sharpness plots
  - (c) Sharpness values per method
3. Cost of computing each method (if its there)
4. Human overhead and difficulty

## Conclusions

Observations about relative accuracies, calibrations, sharpnesses, overhead

## Code availability

Visit [https://github.com/ulissigroup/uncertainty\\_benchmarking](https://github.com/ulissigroup/uncertainty_benchmarking) for the code used to create the results discussed in this paper. The code dependencies are listed inside the repos-

itory.

## **Author information**

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## References

- (1) Tran, K.; Ulissi, Z. W. *Nature Catalysis* **2018**, *1*, 696–703.