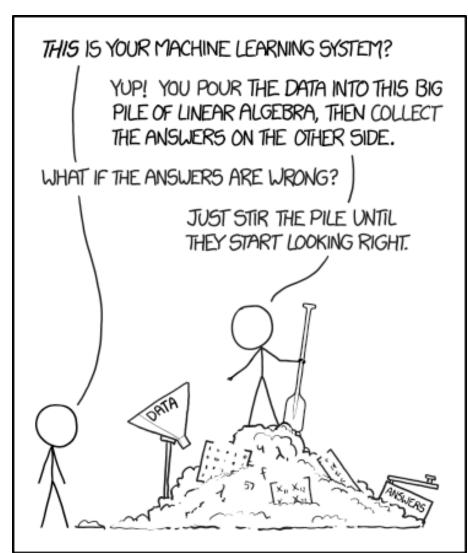# Conclusions and some thoughts to chew

- Designing better materials critical for performance improvement in several applications
  - Computations + AI/ML can significantly accelerate materials design

- Different ways to use ML (or precursors to ML)
  - Regressions (or classifications): predict properties using experimental/calculated properties
  - Interatomic potentials: model larger/longer phenomena on a dynamic lattice
  - Diffusion and language models, transfer learning

- Materials science is a data-limited domain
  - Garbage in = Garbage out; data normalization
  - Real vs. synthetic data
  - What model to choose? Simple models are usually better
  - Choose features carefully: physically intuitive?
  - Don't do ML just because you can (hammer doesn't beget a nail)
  - Construct models with care: overfitting, lack of transferability
  - Test and validate, validate and test, and …

saigautamg@iisc.ac.in; https://sai-mat-group.github.io; https://github.com/sai-mat-group

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