



## Summer 2020 Projects at the USM

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- Development of robust population-based approaches to materials modeling
  - Swarm intelligence
  - Differential Evolution
  - Ant Colony systems

- Maximum-Entropy optimization: From function reconstruction to electronic-structure calculations
  - Total-energy and force calculations
  - Density/function reconstruction from a set of noisy moments
  - Beyond Boltzmann-Gibbs entropy: Tsallis'/Reyni's/generalized  $q$ -entropy
  - Applications of Fisher information in materials modeling

# Example projects – developing ideas

- Bayesian computation in materials modeling
  - Structural inference (of small clusters/disordered solids)
  - Dynamic determination of RMC weights
  - Amorphous graphene/silicene and various other 2-dimensional compounds