Edisonian approach to materials development

- Trial-and-error
- High material and labor cost
- Difficult testing in extreme environments
- Lack of methods to full probe molecular scale behavior

“\textit{I have not failed. I've just found 10,000 ways that won't work}” – Thomas Edison

Computational approach to materials development

- Efficiently explore design space
- Predict material behavior under a wide range of conditions
- Provide physical insight into observed behavior

SUPERIOR high-performance computing cluster
Projects

- Conformable CNG tank
- Computational modeling of internal stresses

**Epoxy molecules**
- Graphene
- O atom
- C atom
- H atom

**Rapid material development**

**Structure-property relationships**

**Computational modeling**