

Data Storage

Data Storage Schema

What data needs to be stored?

Where should we store it?

Molecular Dynamics

input file

Date

structure(s) files

Forcefield files (if not generic)

Forcefield version

MD engine used

MD engine version

Post-analysis script or link

DFT

FEA

Data Storage Diagram

Material Property Schema

Best way to store and label data associated with predicted properties?

Best way to predict confidence level in predicted property?

Development of generic schemas to allow fitting in with Citrine

<https://citrine.io/>

Molecular Dynamics

Link to Stored data

Material property of interest (e.g. Tg)

Metadata tags (material type, composition, etc.)

DFT

FEA

