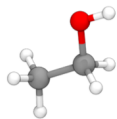


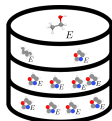
Model training



atomic structure

Electronic
structure
theory method

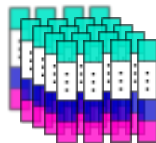
$\rightarrow E \rightarrow$



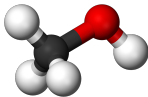
Featurization

data-driven
model

Training



Model deployment



Featurization



\rightarrow

data-driven
model

Energy

Prediction