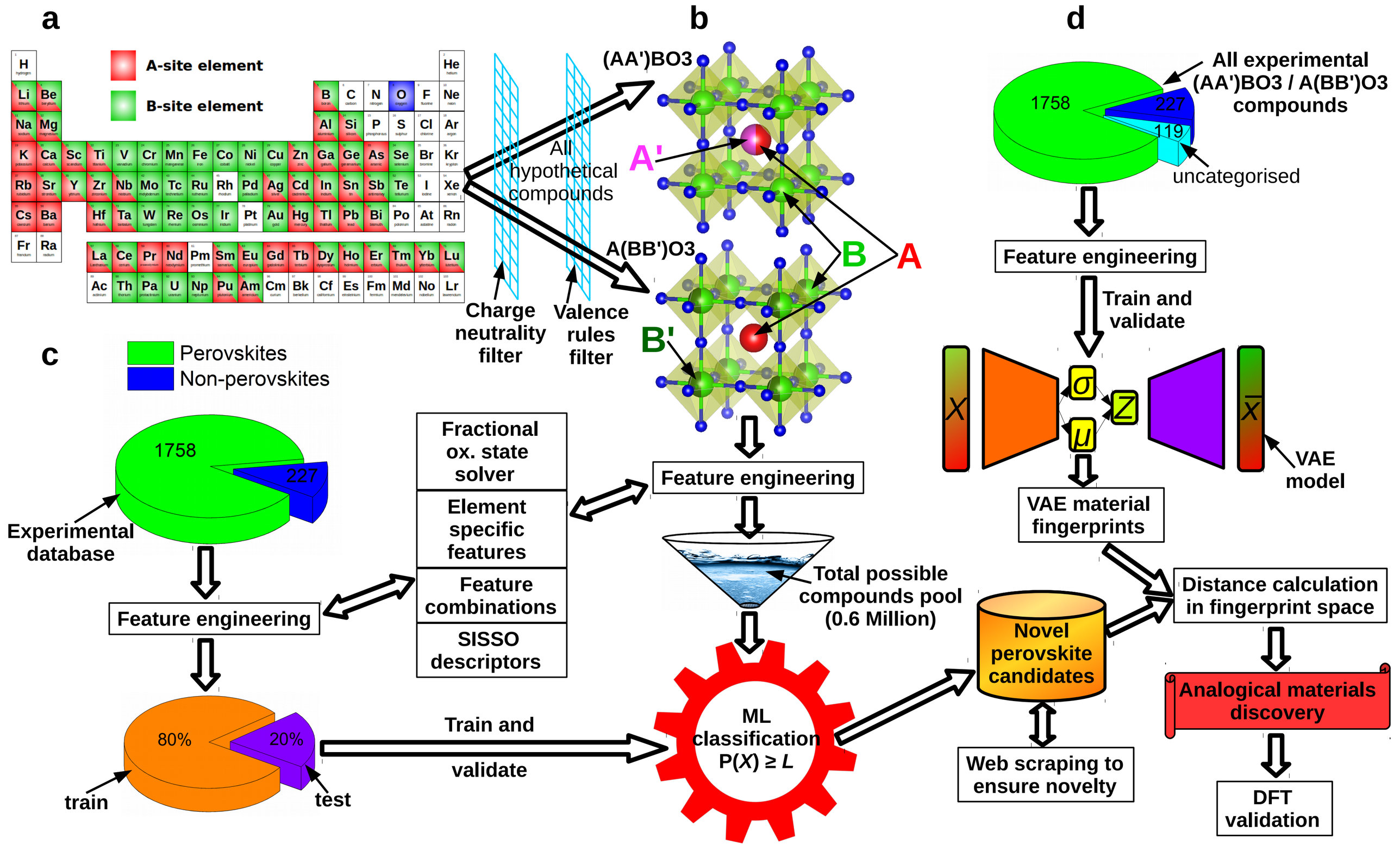
a
A-site element
B-site element
b
(AA')BO3
A(BB')O3
A'
B
A
B'
All hypothetical compounds
Charge neutrality filter
Valence rules filter
d
1758
227
119
All experimental (AA')BO3 / A(BB')O3 compounds
uncategorised
Feature engineering
Train and validate
X
σ
μ
Z
X̄
VAE model
VAE material fingerprints
c
Perovskites
Non-perovskites
1758
227
Experimental database
Feature engineering
80%
20%
train
test
Train and validate
Fractional ox. state solver
Element specific features
Feature combinations
SISSO descriptors
Feature engineering
Total possible compounds pool (0.6 Million)
ML classification P(X) ≥ L
Novel perovskite candidates
Web scraping to ensure novelty
Distance calculation in fingerprint space
Analogical materials discovery
DFT validation