Deep neural nets
can help double the battery life of your phone

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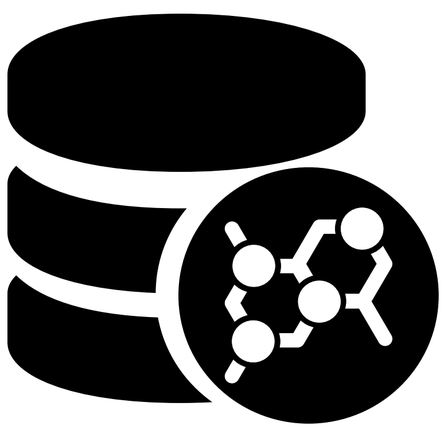
by speeding up the search for new battery materials†

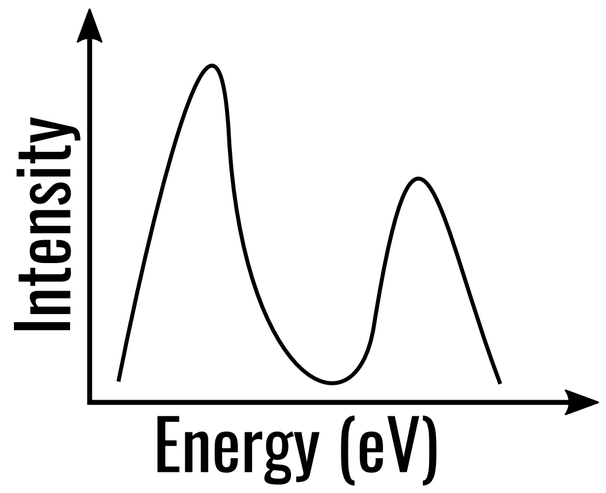
But first, searching for new materials 101 : material characterization



Molecular database

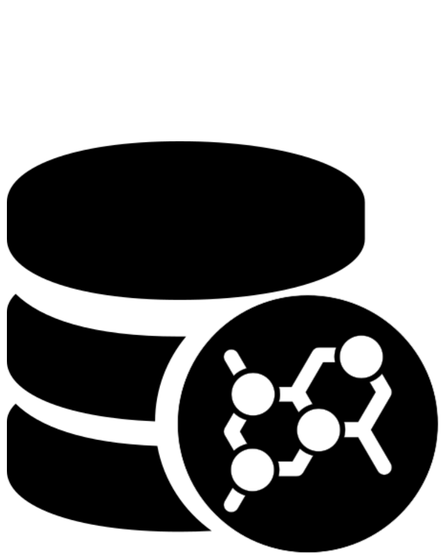
Run simulations modelling complex atomic interactions

Simulations very slow.
Took us one month to compute spectra for a dataset of 132K molecules

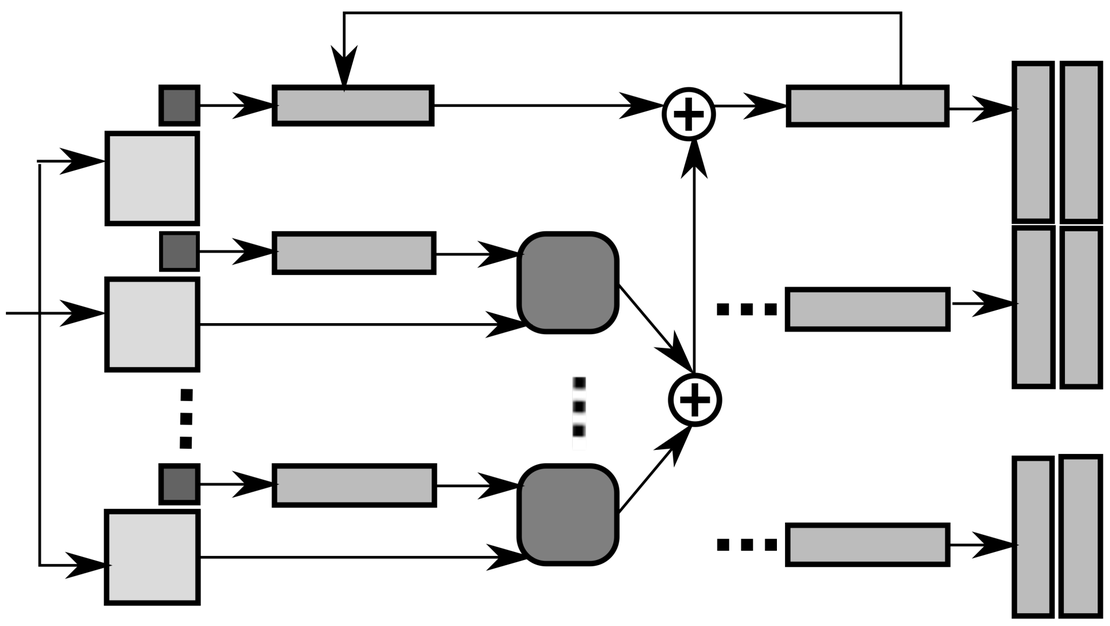


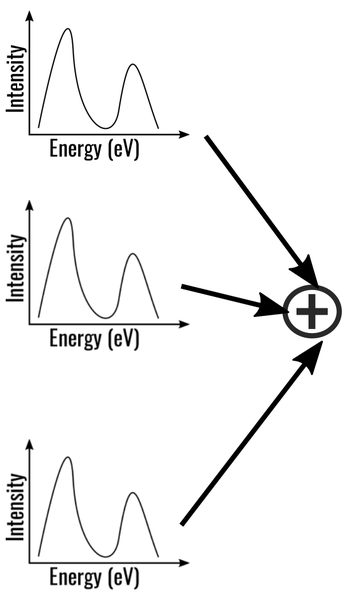
Compute spectra for characterizing the molecules

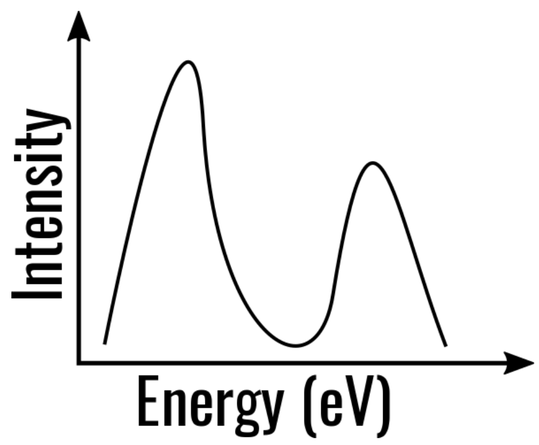
Replace slow simulations with custom designed* neural nets (for inference)



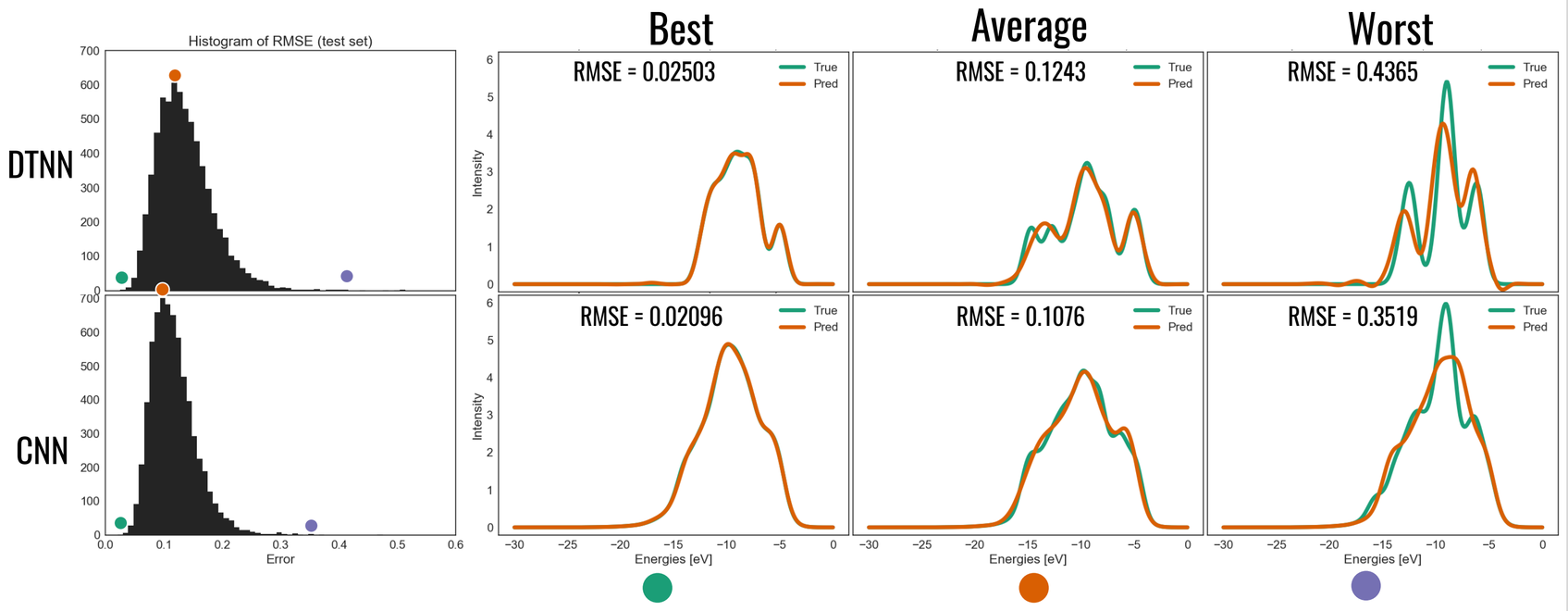
Molecular database







Results and contact details



Deep Learning for Predicting Molecular Electronic Properties,
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† One possible way to double the battery life of phones.
* Modified from deep tensor neural networks (Schutt et.al 2017)