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Constructing interatomic potentials from first principles using machine learning: the example of tungsten

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This talk will report on our recent progress with generating force fields (interatomic potentials) with first principles accuracy using machine learning, specifically Gaussian process regression. The three key ingredients are: a representation, an interpolation scheme, and a protocol for generating data. A lot of progress was made on the first two in our group and others in the last few years, and now we are turning our attention to the much less well defined problem of what needs to be in a database of first principles calculations in order to recover specific materials properties using the interpolated potential. The first illustration will be on tungsten and if time allows on water (in cluster, liquid and ice forms).