Contribution ID: **70** Type: **not specified**

An Invariant of the xTB initial Hamiltonian as a chemical Descriptor for DFT regression

We show that the first-guess electronic Hamiltonian from xTB (extended tight-binding) calculations can be used as a chemical descriptor with all common invariances (i.e. translation, rotation, reflection, and permutation) via simple orthonormal matrix transformations. Artificial neural networks (ANNs) were trained on a labeled dataset of water dimer clusters with the aforementioned first-guess Hamiltonian matrices as inputs to evaluate their potential as descriptors for a regression of the converged SCF Hamiltonian and the corresponding electron density. Our tests using linear regression resulted in a band-structure energy mean absolute error of 15.02 mHa with our invariances applied compared to 73.58 mHa without the invariances.

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Session Classification: Poster flash talks