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Artificial Neural Network-Based Density Functionals for transition Metal Complexes

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Despite its many successes, the implementation of density-functional theory (DFT) still faces several challenges that limit its predictive power and applicability. Recently, several studies have shown how DFT can benefit from machine learning techniques where the functional “learns itself” from a given set of high quality data. This philosophy is adopted in our work to push the accuracy of DFT in the prediction of challenging electronic structure properties. In my talk, I will describe our efforts in the development of new exchange and correlation functionals that achieve good accuracy in the prediction of transition metal complexes. These physically constrained-artificial neural network (ANN) functionals are trained with a small set of of energies and electronic densities using a non-gradient based bio-inspired training method adapted from Particle Swarm Algorithm. Our results show that a robust meta-GGA functional developed in this way can outperform most known density functionals in the prediction of adiabatic energy differences, dissociation energies, and reaction barriers, for a large variety of molecules and ions, thus demonstrating its transferability.