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FFLUX: Adding Dispersion to a Quantum Mechanical Force-Field through Machine Learning and Electronic Correlation

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Abstract: The state in which force fields are used in molecular dynamics has changed very little over the past 30 years. The most energy-transferable way to describe an atom within a system is through Quantum Chemical Topology[1] (QCT). A force field based on QCT emerges as an attractive alternative to provide atomistic energies for molecular dynamics simulations. We present, for the first time, an innovative method for predicting the dynamic electron correlation (Dispersion) energy of an atom or a bond in a molecule. Our approach uses the machine learning method Kriging (Gaussian process regression with a non-zero mean function) to predict these dynamic electron correlation energy contributions. The true energy values are calculated by partitioning the MP2 two-particle density-matrix via the Interacting Quantum Atoms[2] (IQA) procedure. In principle, we hope to use Dynamic Correlation to add Dispersion energies our *ab initio* force-fields, named **FFLUX**[3]. We show some results:

I) We show the first *ab initio* Lennard-Jones parameter B=514.6, obtained through IQA and correlation energies for the water dimer (Fig .1a and b).

II) Also, we Machine learn the electronic correlation of a GLU-ALA helix, predicting the electronic correlation of around 900 geometries, from 190 training points. The predictions of the helix have a maximum absolute error below 5.3 kJ/mol with R-square equal to 0.997 (Fig 1.c).

III) Finally, we can calculate atomic and bond correlation energies for amino acids in explicit solvation. The O…H hydrogen bond interactions are negative and the O…O and O…N are positive, causing a partial cancelation in the correlation energy of the hydrogen bond(Fig 1d).

a)

c)

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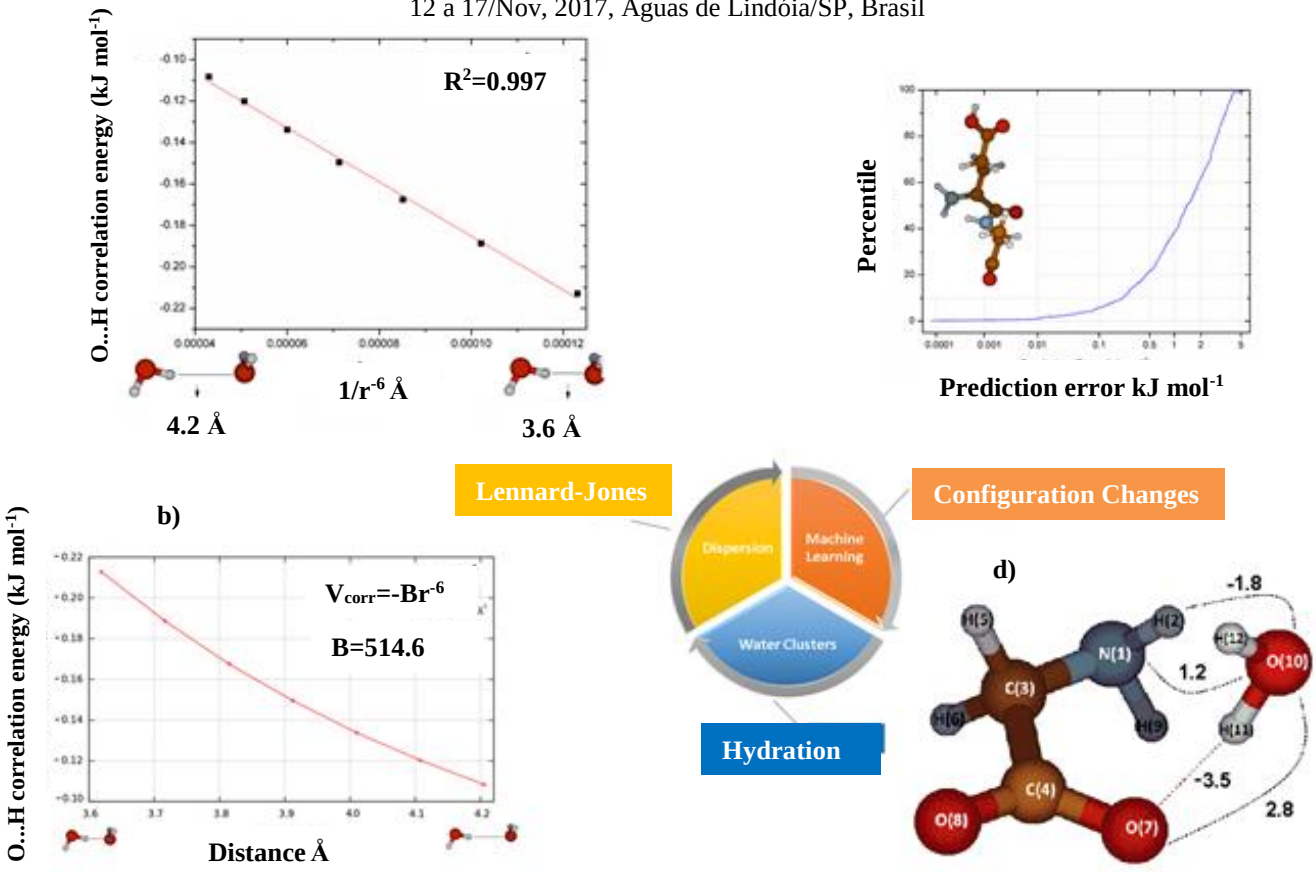

Figure 1. a) The correlation energy (kJ mol^{-1}) of the hydrogen bond ($H_2O\ldots H_2O$) vs $1/r^6$ distance in Angstroms for the water dimer at the MP4/6-31G++(2d,2p) b) The correlation energy (kJ mol^{-1}) of the hydrogen bond ($H_2O\ldots H_2O$) vs distance in Angstroms for the water dimer at the MP4/6-31G++(2d,2p) c) The S-curve for the predictions of the total ECE of the alanine-glutamic acid helix derived from kriging.. And d) Optimized geometry of glycine hydrated with one water molecule, with some hydrogen bond correlation values

Key-words: ab initio force-field, peptides, machine learning, dispersion energy
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