A fully nonlocal DFT framework for the construction of novel approximations

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Density Functional Theory (DFT) is the fundamental building block of the successes of theoretical and computational chemistry in understanding and guiding experiments. Despite the widespread success of DFT approximations (DFAs), there are still situations when they can give even qualitative failures. Most notables failures are encountered when DFAs are applied to strongly correlated systems and systems that exhibit significant self-interaction errors. The inability of DFAs to describe such systems and processes hampers their overall predictive power and usability in chemistry.

In his talk, I will discuss how the problem of strong correlation within DFT can be addressed by using a novel framework for the construction of a new generation of DFAs. [1,2] The methodology is applied to simple, yet illustrative chemical systems and processes. These results show that the new DFT framework has a great potential for simultaneously addressing both the strong correlation [2] and dispersion interactions problems within DFT [3]. Finally, directions for future improvements [1,4] aiming at bringing the methodology to desired chemical accuracy will also be outlined.

References

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