Making the zoo of Density Functional Theory methods more accessible: a story of contributions to ground and excited state DFT

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First of all, I would like to express my gratitude to the APATCC for awarding me the 2022 Pople Medal. In my medal plenary talk, I will provide snapshots of my group's contributions towards making the zoo of Density Functional Theory (DFT) methods more accessible to users while simultaneously giving useful insights to developers.

I will begin by giving a brief overview of our work on the GMTKN55 database for General Main Group Thermochemistry, Kinetics and Noncovalent Interactions by highlighting how the insights for ground-state DFT methods in this space goes beyond the original GMTKN55 publication,[1] with my group having created and analysed data for more than 350 dispersion-corrected and uncorrected functionals.[2]

The main part of my presentation will then deal with time-dependent DFT (TD-DFT) with special emphasis on double-hybrid density functionals (DHDFs). Earlier work has shown DHDFs to be accurate candidates for the calculation of excitation energies.[3] However, the older generation of DHDFs still failed to describe long-range excitations, such as Rydberg and the more important charge-transfer excitations. This presentation discusses our range-separated DHDFs,[4] which belong to some of the most balanced, robust and accurate DFT methods for excitation energy calculations in organic molecules,[4,5] incl. open-shell systems[6] and aromatic excimers.[7]

References

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