Fukui function calculation along electronic dynamics simulations

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Characterizing the reactivity of molecules subjected to radiation of varying energies remains an objective in theoretical chemistry. In particular, the advent of ultrafast pump-probe technologies on femtosecond and even attosecond scales is bringing to light reactive processes that are stimulating to theoretical chemists. In this context, the conceptual DFT descriptors that have proven their relevance in stationary DFT [1] deserve to be adapted to excited electronic states [2].

In this presentation, we propose an original extension of Fukui function computation along RT-TD-DFT (Real-Time Time Dependent Density Functional Theory) simulations of electronic dynamics. Our implementation is based on Auxiliary DFT using the deMon2k software. The electronic density is propagated according to the time-dependent Kohn-Sham framework with the use of variational density fitting [3]. Irradiation by UV or extreme UV external electric fields or by rapid ions are accessible to the code. Examples of applications for radiation chemistry or attosecond spectroscopies will be shown.

References

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