PRODUCT BASIS SET IN TDDFT: MOLECULAR ABSORPTION SPECTRA WITHIN LINEAR RESPONSE.

Peter Koval and Dietrich Foerster
CPMOH - France

We propose a new basis set [1] and corresponding method [2] to calculate of the Kohn-Sham density response function.
Computational cost of our method scales comparatively cheaply with the number of atoms N.

Here we discuss the application of our technique to the computation of molecular absorption spectra. Spectra are calculated directly in O(N**2) operations from the Gross-Petersilka-Gossmann equations [3].

References:

[1] Foerster~D, J. Chem. Phys. 128 034108 (2008)

[2] Foerster~D, Phys. Rev. B 72 073106 (2005)

[3] Petersilka M, Gossmann U J and Gross E K U, Phys. Rev. Lett. 76 1212 (1996)