Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Ultrafast Nonadiabatic Dynamics Probed by Nitrogen K-edge Absorption Spectroscopy: Supporting Information

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List of Figures

S1 Populations Kinetics

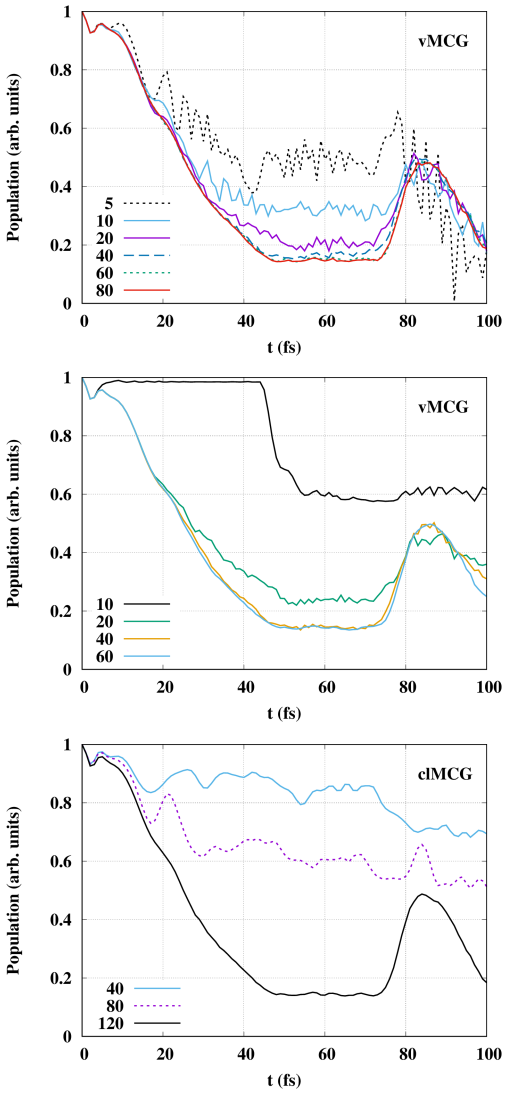

Figure S1: The population kinetics of the S_2 state for vMCG singlet-set (upper), vMCG multi-set (middle) and clMCG (lower) simulations. The legend in each case shows the number of GBFs and in each case the largest number converges onto the results obtained using quantum dynamics within the multi-configuraitonal time-depdendent Hartree method, as shown in ref. [1].

S2 Time-resolved XANES

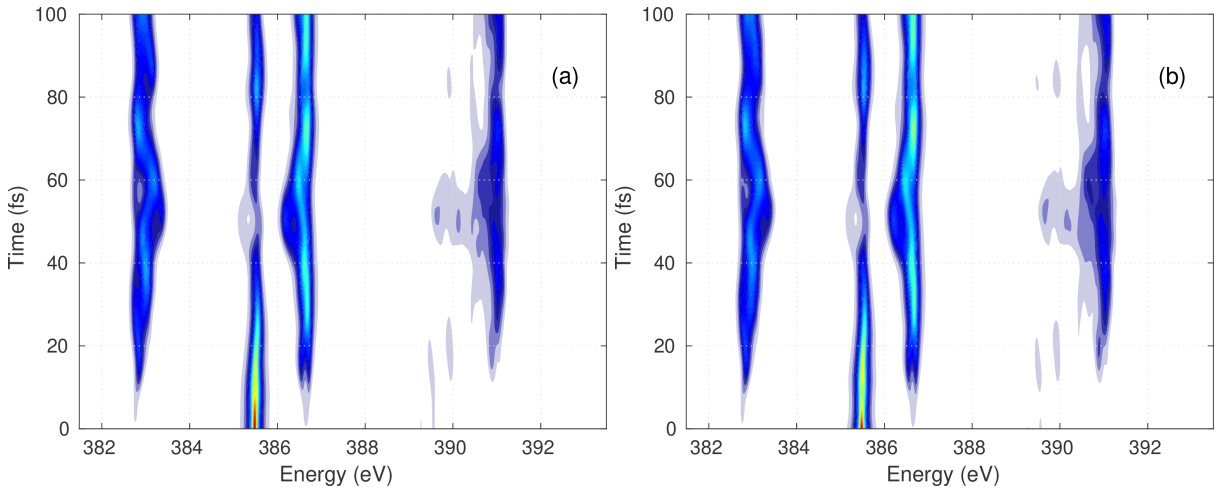

Figure S2: The time-resolved nitrogen K-edge XANES spectra of pyrazine calculated using MOM/TDDFT with 40 GBFs (left) and 60 GBFs (right) in the single-set formalism using vMCG.

References

[1] GW Richings, I. Polyak, KE Spinlove, GA Worth, I. Burghardt, and B. Lasorne. *Int. Rev. Phys. Chem.*, 2015, **34**, 269–308