Laser-induced electron dynamics including photoionization: A heuristic model within TD-CI theory

Stefan Klinkusch, Tillmann Klamroth, and Peter Saalfrank

Institut für Chemie, Universität Potsdam Karl-Liebknecht-Str. 24-25, D-14476 Potsdam, Germany

We report simulations of laser-pulse driven many-electron dynamics by means of a simple, heuristic extension of the time-dependent configuration interaction singles (TD-CIS) approach. The extension allows for the treatment of ionizing states as non-stationary states with a finite, energy-dependent lifetime to account for above-threshold ionization losses in laser-driven many-electron dynamics. The extended TD-CIS method is applied to the following specific examples: (i) State-to-state transitions in the LiCN molecule which correspond to intramolecular charge transfer and (ii) creation of electronic wavepackets in LiCN including wavepacket analysis by pump-probe spectroscopy.

Literature:

T. Klamroth, Phys. Rev. B 68, 245421 (2003) and references therein.

P. Krause, T. Klamroth, and P. Saalfrank, J. Chem. Phys. 123, 074105 (2005).

S. Klinkusch, T. Klamroth, and P. Saalfrank, *Phys. Chem. Chem. Phys.* **11**, 3875 (2009).

S. Klinkusch, P. Saalfrank, and T. Klamroth, J. Chem. Phys. 131, 114304 (2009).