Simulations of time-resolved photoelectron spectra using extended time-dependent configuration interaction methods

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We report simulations of time-resolved photoelectron spectra (TRPES) of gold nanoclusters (Au_7^- and Au_9^-) using extended time-dependent configuration interaction (TD-CI) methods [1] and perturbation theory. These methods have been extended to calculate the effects of photoionization [2] and dissipative effects (mainly non-radative or radiative relaxation, such as fluorescence and internal conversion, and dephasing) [3, 4]. In this scheme, we try also to include nuclear dynamics to simulate a transformation among the three isomers of the respective nanoclusters. The dynamical methods are then used to simulate pump-probe spectra according to an experiment performed by Stanzel *et al.* [5].

References

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