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Molecular double-core-hole-state formation in the XFEL regime

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The unprecedented radiation intensity of x-ray free electron lasers (XFELs) offers the possibility to create double-core-hole (DCH) states with a single femtosecond pulse via sequential two-photon absorption [1,2]. This opens the way to develop powerful tools for chemical analysis such as the x-ray two-photon photoelectron spectroscopy [3]. In this context, we have recently developed a complete time-dependent quantum description taking into account x-ray absorption, nuclear dynamics and Auger decay [4]. Using this model, we have assessed the impact of the nuclear dynamics on DCH processes in the CO molecule. Our study shows that sequential absorption of two x-ray photons modifies significantly the photoelectron spectra compared to direct single photon absorption. Depending on the shape of the potential energy curves involved in the processes, different vibrational levels may be favored. Furthermore, when the final state is dissociative, the electron spectrum is further broaden and blue-shifted in the two-photon process. In the talk I will i) summarize the main ingredients of our quantum approach and ii) report on the results of our study on CO and its relevance in the context of XFEL.
[1] N. Rohringer and R. Santra, Phys. Rev. A 76, 033416 (2007).
[2] L. Young et al., Nature (London) 466, 56 (2010).
[3] R. Santra, N. V. Kryzhevoi, and L. S. Cederbaum, Phys. Rev. Lett. 103, 013002 (2009).
[4] S. Oberli, N. Sisourat, P. Selles, and S. Carniato, Phys. Rev. A 97, 013406 (2018).

Choix de session parallèle

6.4 Résultats scientifiques récents obtenus avec les XFEL

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