CFEL SCIENCE

SEMINAR

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CFEL-bldg. 99, seminar room IV

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From atoms to molecules in intense x rays: a small step?

X-ray science is undergoing one of its greatest revolutions to date with the advent of x-ray free electron lasers (FELs). A thorough theoretical understanding of the underlying physics of the interaction of matter with FEL x rays is paramount for future progress in the field. Our theoretical work relates to experiments with neon atoms and nitrogen molecules (N_2) in gas phase exposed to intense and ultrafast x rays from the Linac Coherent Light Source (LCLS) in Menlo Park, California, USA. We treat the electronic structure of neon using a relativistic multiconfiguration approach. The interaction with the x rays is described in rate-equation approximation which includes two-electron emission; ion yields and photon yields are determined. To understand the mechanisms of the interaction, a path analysis is devised which allows us to investigate what sequences of photoionization and decay processes lead to a specific configuration and with what probability. Thereby we uncover a connection to the mathematics of graph theory and formal languages. To study the quantum dynamics of N_2, we set out from a rate-equation description of a nitrogen atom; molecular effects are then incorporated as follows: First, we devise phenomenological models: a single atom, a symmetric-sharing, and a fragmentation-matrix model. Second, molecular rate equations are developed. With this we calculate ion yields and the average charge state and explain the effect of frustrated absorption. Prospects for future research are highlighted.

References

[1] Buth, C., Beerwerth, R., Obaid, R., Berrah, N., Cederbaum, L. S. & Fritzsche, S. Neon in ultrashort and intense x rays from free-electron lasers. arXiv:1705.07521 (2017).

[2] Buth, C., Liu, J.-C., Chen, M. H., Cryan, J. P., Fang, L., Glownia, J. M., Hoener, M., Coffee, R. N. & Berrah, N. Ultrafast absorption of intense x rays by nitrogen molecules. J. Chem. Phys. 136, 214310 (2012).

[3] Liu, J.-C., Berrah, N., Cederbaum, L. S., Cryan, J. P., Glownia, J. M., Schafer, K. J. & Buth, C. Rate equations for nitrogen molecules in ultrashort and intense x-ray pulses. J. Phys. B 49, 75602 (2016).

Host: Robin Santra – CFEL-DESY Theory Division