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XMDYN: Modeling radiation damage of XFEL irradiated samples

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High-resolution x-ray imaging of nanosize biological samples is one of the most important goals of the research with X-ray free electron lasers (XFEL) [1]. Outstanding results have already been achieved in serial nano-crystallography [2]. There has been also a significant progress in the field of single particle imaging [3]. However, radiation damage is still a limiting factor, in particular for non-periodic objects. This requires thorough theoretical investigations of the time evolution of the irradiated samples.

Here we report on XMDYN [4], our molecular-dynamics based tool to model the dynamics of finite samples irradiated by high intensity x-ray pulses. First we describe the theoretical approach used. To validate the model we then show predictions of the model as compared to experimental results. New developments such as the on-the-fly connection to the atomic physics XATOM toolkit [5] enabling accurate treatment of heavy elements and a possible code extension towards large-scale calculation are also discussed.

[1] R. Neutze, R. Wouts, D. van der Spoel, E. Weckert and J. Hajdu, Nature 406, 752 (2000)
[2] L. Redecke et al. Science 339, 227 (2013).
[3] M. M. Seibert et al. Nature 470, 78 (2011)
[4] Z. Jurek, B. Ziaja, and R. Santra, XMDYN (CFEL, DESY, Hamburg, Germany, 2013).
[5] S.-K Son and R. Santra, XATOM an integrated toolkit for X-ray and atomic physics. (CFEL, DESY, Hamburg, Germany, 2011).

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