Abstract Submitted
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Structures of heterogeneous systems determined using XFEL pulses in the face of radiation damage[1] LINDA YOUNG, PHAY HO, CHRIS KNIGHT, CHRISTOPH BOSTEDT, Argonne National Laboratory, GYULA FAIGL, MIKLOS TEGZE, Hungarian Academy of Sciences — Intense, femtosecond x-ray free-electron laser pulses are a promising tool for studying the structure and dynamics of complex systems at atomic resolution. Our previous efforts, using an atomistic quantum/classical model to track the dynamical evolution of ions and electrons throughout a femtosecond x-ray pulse and out to picosecond timescales, focused on quantifying the effects of radiation damage on homogeneous rare gas clusters for imaging applications in an ideal situation. In these studies, the entire 3D Q-space scattering pattern was computed and available for reconstruction of the initial structure. However, a realistic representation of an experiment would feature a collection of noisy 2D scattering patterns, from which orientation would first be required to generate the 3D Q-space distribution from which solution of the phase problem and reconstruction would then proceed. We will present the first results of these efforts on heterogeneous systems.

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Linda Young
Argonne Natl Lab

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