

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Manifold-embedding methods for extracting continuous conformational ensembles of biological molecules from single-particle measurements using X-ray Free Electron Lasers.¹ JEREMY COPPERMAN, AHMAD HOSSEINIZADEH, GHONCHEH MASHAYEKHI, PETER SCHWANDER, ALI DASHTI, RUSSELL FUNG, ABBAS OURMAZD, University of Wisconsin-Milwaukee, BIOXFEL COLLABORATION — A novel machine-learning approach allows us to navigate the high-dimensional space of single-particle XFEL scattering data. This technique can be used to map continuous conformational changes in biological systems, and to determine the energy landscape associated with such changes. With the extremely large datasets expected from high repetition-rate XFELs about to enter service, this approach promises unprecedented access to rare, rate-limiting conformations energetically far above the thermal bath.

¹Supported by the US Department of Energy, Office of Science, Basic Energy Sciences under award DE-SC0002164, and by the US National Science Foundation under awards STC 1231306.

Jeremy Copperman
University of Wisconsin-Milwaukee

Date submitted: 11 Nov 2016

Electronic form version 1.4