Contribution ID: **8** Type: **not specified**

Controlling protein orientation using strong electric fields: perspectives for single particle imaging

Thursday, October 14, 2021 10:50 AM (25 minutes)

Single particle imaging is a set of emerging techniques that utilize ultrashort and ultraintense X-ray pulses to generate diffraction from single isolated particles in the gas phase to determine their structures. One of the largest difficulties in realizing this goal is the unknown orientation of the individual sample molecules at the time of exposure. The orientation recovery process requires computationally demanding algorithms that in some cases are unable to find the correct solution, making structure determination impossible in those cases. Preorientation of the molecules using external electric fields has been identified as a possible solution to this problem.
Using molecular dynamics simulations, we identify a range of electric field strengths where proteins become oriented without losing their structure. Moreover, for a number of experimentally relevant cases, we show that structure determination is possible only when orientation information is included in the orientation-recovery process. We conclude that non-destructive field orientation of intact proteins is feasible and that it enables a range of new structural investigations with single particle imaging.

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Session Classification: AQUA