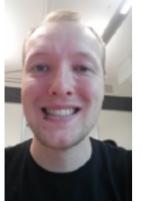
Summary

- Rare events are a difficult, but important, challenge for molecular simulation
- Path sampling is a powerful tool for the study of rare events
- Path sampling gave us insight into why the Q61L mutant of K-Ras causes cancer
- LAMMPS users can use OpenPathSampling to perform path sampling simulations

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K-Ras







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