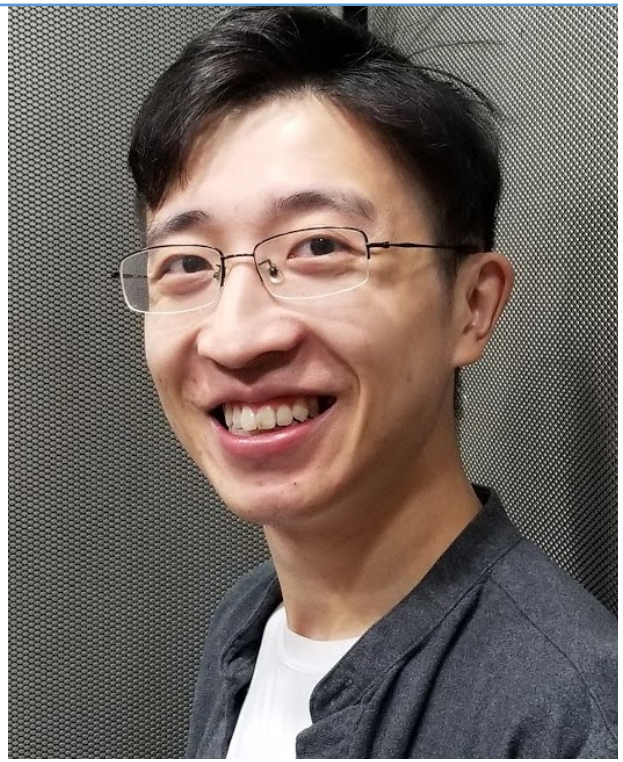
Thesis Defense in Chemistry

Tuesday, October 1, 2019 at 1:00pm
Room 428 Pupin
Please note location



Loop prediction and homology modeling with high resolution

Presented by Tianchuan Xu, Friesner Group

Abstract: Knowledge of protein 3D structure is integral to structure-based drug discovery. To achieve robust homology modeling with atomic-level accuracy, reliable loop predictions are required. I will introduce Protein Local Optimization Program (PLOP) that is designed to produce native-like predictions on loop regions in homology modeling. Promising results are obtained in predicting antibody H3 loop, notorious for its conformational diversity. I will also discuss PLOP-related ongoing projects, including GPU acceleration and deep learning implementation.

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