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ETD Submission Details for Madilyn Paul

Basic Details

Title: Development and application of computational tools for organic molecular structure prediction from small molecule crystal structure determination to polymer persistence length.

Author(s): Madilyn E Paul Primary Language: English
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Student Notes to Administrator:

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Degree/Department Information

Degree Date: Nov, 2024

Degree Awarded: Doctor of Philosophy in Materials Science and Engineering

Year Manuscript Completed: 2024

Department: Materials Science and Engineering **Advisor/Supervisor/Committee Chair:** Eric Jankowski

Committee Members: Scott Phillips, Oliviero Andreussi, Frank Willmore

Subject Categories

Materials Science [0794] - primary

Keywords

Conjugated Polymers
Density Functional Theory
Molecular Dynamics



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