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**pysimm: A Python Package for Simulation of Molecular Systems**

MICHAEL FORTUNATO, CORAY COLINA, University of Florida — pysimm, short for python simulation interface for molecular modeling, is a python package designed to facilitate the structure generation and simulation of molecular systems through convenient and programmatic access to object-oriented representations of molecular system data. This poster presents core features of pysimm and design philosophies that highlight a generalized methodology for incorporation of third-party software packages through API interfaces. The integration with the LAMMPS simulation package is explained to demonstrate this methodology. pysimm began as a back-end python library that powered a cloud-based application on nanohub.org for amorphous polymer simulation. The extension from a specific application library to general purpose simulation interface is explained. Additionally, this poster highlights the rapid development of new applications to construct polymer chains capable of controlling chain morphology such as molecular weight distribution and monomer composition.

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