[P23] Molpher-lib: software library for systematic chemical space exploration

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Molpher is a user-targeted software that implements a new method for *in silico* exploration of chemical space called molecular morphing [1]. Although Molpher is a very useful on its own, it still suffers from a few shortcomings and disadvantages; for example, the low flexibility of its source code makes it hard to make changes to the algorithm or extending the program with new features. In this work, we introduce a software library, Molpher-lib, which is based on the original implementation of Molpher, but aims to offer more flexibility to the users by enabling easy modifications to the underlying exploration algorithm, providing better access to the generated data during runtime and adding more configuration options. In order to eliminate the shortcomings of Molpher, its C++ code was refactored and rewritten to create a more modular architecture whose functionality could be easily exposed through an application programming interface (API). This feature rich API is also exposed to the Python programming language, which is very popular in the scientific community. Therefore, the library maintains the speed of the original implementation, but at the same time makes it very easy to integrate molecular morphing into existing applications, directly affect the exploration process by writing code in a high-level programming language and analyze the results with ease using tools that most scientists are already familiar with.

Bibliography:

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