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ChemHTPS - A virtual high-throughput screening program suite for the chemical and materials sciences MOHAMMAD ATIF FAIZ AFZAL, WILLIAM EVANGELISTA, JOHANNES HACHMANN, State University of New York, University at Buffalo — The discovery of new compounds, materials, and chemical reactions with exceptional properties is the key for the grand challenges in innovation, energy and sustainability. This process can be dramatically accelerated by means of the virtual high-throughput screening (HTPS) of large-scale candidate libraries. The resulting data can further be used to study the underlying structure-property relationships and thus facilitate rational design capability. This approach has been extensively used for many years in the drug discovery community. However, the lack of openly available virtual HTPS tools is limiting the use of these techniques in various other applications such as photovoltaics, optoelectronics, and catalysis. Thus, we developed ChemHTPS, a general-purpose, comprehensive and user-friendly suite, that will allow users to efficiently perform large in silico modeling studies and high-throughput analyses in these applications. ChemHTPS also includes a massively parallel molecular library generator which offers a multitude of options to customize and restrict the scope of the enumerated chemical space and thus tailor it for the demands of specific applications. To streamline the non-combinatorial exploration of chemical space, we incorporate genetic algorithms into the framework. In addition to implementing smarter algorithms, we also focus on the ease of use, workflow, and code integration to make this technology more accessible to the community.

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