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Open Boundary Conditions for Quantum Models in Fluids

An NEGF-adapted algorithm offers a reliable method for predicting the influence of formulation, temperature, and shelf life on drug molecules, saving resources in R&D.

Researchers at Purdue University have developed an algorithm that adapts NEGF to molecular chemistry. This modeling technique would be valuable to general chemistry companies and pharmaceutical companies. In particular, pharmaceutical R&D would benefit from this technology, since it allows for predicting the influence of formulation, temperature, shelf life, etc., on the drug molecules. It can thereby avoid unrealistic predictions and save resources otherwise wasted with futile experiments.

Advantages:

-Predicting molecular properties

-More reliable than existing tools

-Easy to run

Potential Applications:

-Chemistry companies

-Pharmaceutical companies

TRL: 3

Intellectual Property:

Provisional-Patent, 2017-06-29, United States | Copyright, 2017-06-29, United States | PCT-Patent, 2018-06-29, WO | NATL-Patent, 2019-12-19, United States | CON-Patent, 2022-11-18, United States | CIP-Patent, 2023-01-27, United States

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temperature influence, shelf life prediction, molecular property prediction, reliable modeling tool, chemistry company solution, Algorithm, Chemical Synthesis, Chemistry and Chemical Analysis, Molecular Chemistry, Molecules, Quantum