REACTER: A Versatile Tool for Large-Scale Reactive Molecular Dynamics

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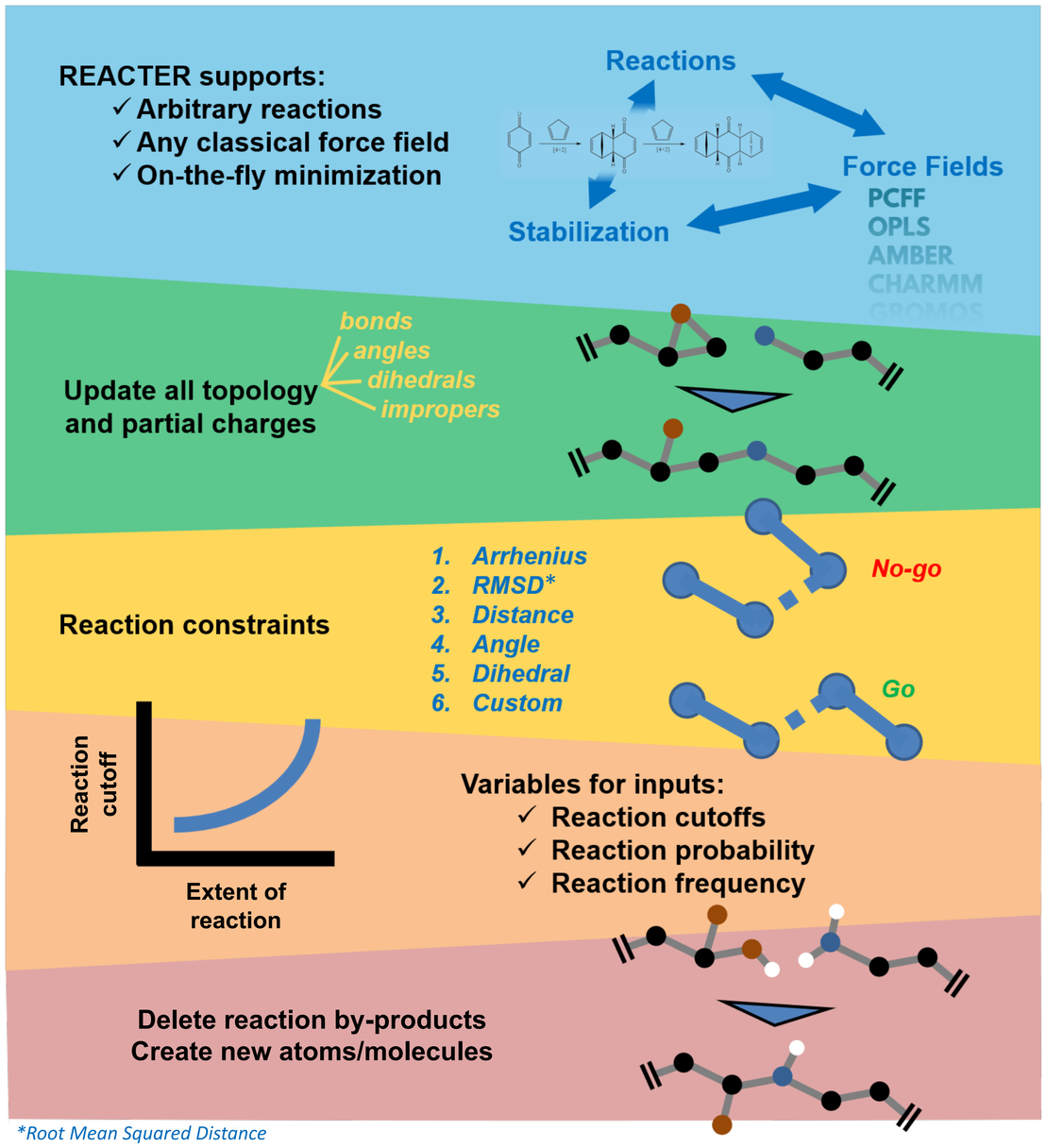
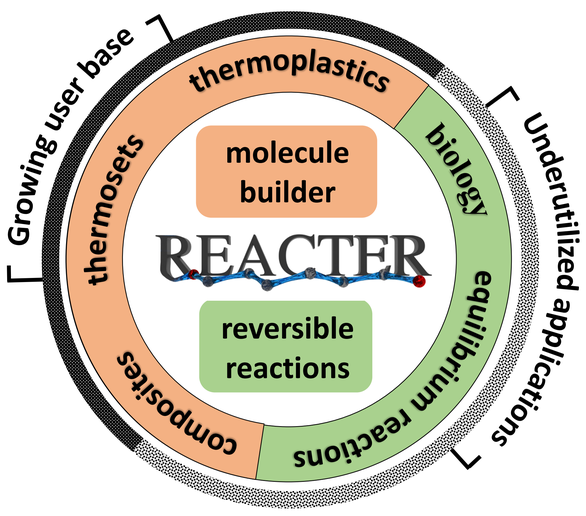
All Images Credit NASA.

REACTER is a protocol for modeling chemical reactions in classical molecular dynamics simulations.



*Root Mean Squared Distance



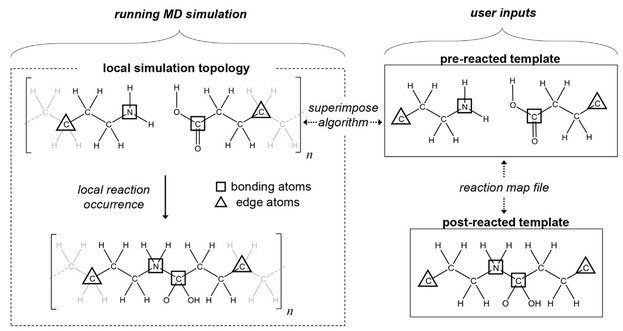
Features In Progress:

1) More flexible reaction templates.
2) Automatic typing of new interactions.
3) Machine-learned reaction constraints.

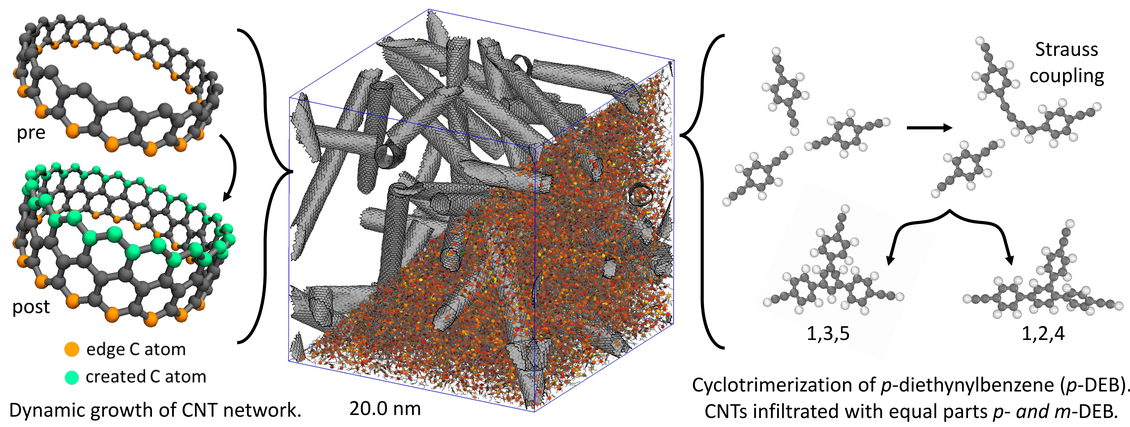
reacter.org

An Example Workflow: Making and Breaking Polymer/Carbon Nanotube (CNT) Composites

The core algorithm of the REACTER protocol identifies reaction sites, which are converted to post-reaction topologies. Implemented in LAMMPs as '*fix bond/react*'.



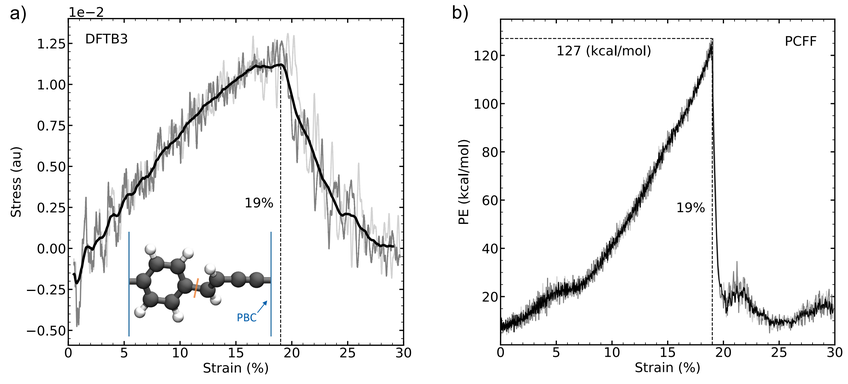
Reaction templates used for CNT growth and *in situ* polymerization.



Dynamic growth of CNT network.

Cyclotrimerization of *p*-diethynylbenzene (*p*-DEB). CNTs infiltrated with equal parts *p- and m*-DEB.

Chain scission enabled using DFT-parameterized strain-at-failure.



a) Tight-binding density functional (DFT) theory determines the ultimate strain and weakest bond (orange slash).

b) Custom reaction constraint has access to internal LAMMPS variables. The total potential energy of reacting atoms is used to reproduce the ultimate strain.

Cured CNT composite subjected to massive uniaxial strain.