

# The Role of Hypervelocity Impacts in Prebiotic Chemistry: Secondary Impact and Planetary Gravity

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#### **Hypervelocity Ice Impact**

- Our recent reactive molecular dynamics simulation study has successfully integrated chemistry and dynamics enabling investigation of the effect of impact velocity to chemical reactions
- Starting with the hypervelocity impact of an H<sub>2</sub>O ice nanograin, we've identified two **velocity thresholds** for: (a) **hydrogen bonds** between water molecules, and (b) **covalent bonds** within a water molecule.

### Primary Impact VS Secondary Impact

- Despite often being overlooked, secondary impacts are crucial due to their high frequency.
- Each primary impact produces 100,000 secondary impacts estimated by Costello et al. [1]
- The velocity of secondary impacts, controlled by a planet's gravity, plays a crucial role in determining the energy available for these prebiotic reactions, highlighting their importance in astrobiology studies.

### Next-gen Computational Chemistry!

- Automatic Chemical Reaction Network Exploration: Machine learning techniques automate the exploration of chemical reactions, efficiently predicting feasible reactions and streamlining chemical discovery.
- Ab-initio nanoreactor [2]: Machine learning interatomic potentials (MLIPs) offer a cost-effective substitute for the resource-intensive ab initio simulations. Expanding more possibility for prebiotic reactions.







## **Reference:**

[1] Costello, E. S., et al. Nature Astronomy 5.9 (2021): 951-956.
[2] Wang, Lee-Ping, et al. Nature chemistry 6.12 (2014): 1044-1048.

