BLUE WATERS
SUSTAINED PETASCALE COMPUTING

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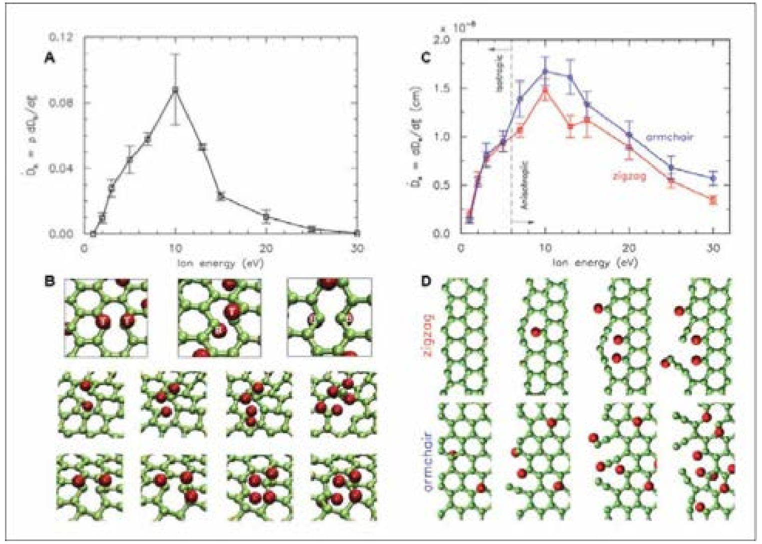


a) Steady state basal plane etching rate versus ion energy for monolayer graphene; b) Mechanism of etching showing the three possible configurations of damage nucleation and progression; c) Etching rates of the zigzag and armchair configurations versus ion energy; and d) Mechanism of etching for zigzag and armchair edges.

# SCALABLE NANOPATTERNING OF GRAPHENE BY HYDROGEN- PLASMA ETCHING

## Research Challenge

While there exists ample experimental evidence for the patterning of graphene by hydrogen-plasma treatment, the reported etching reactions and the resulting graphene nanostructures have been vastly different. The complete parameter space of substrate temperature, ion energy, and incident flux has not been systematically studied due to the cost limitations of plasma experiments.

## Methods & Codes

The team performed length-scale bridging by delineating the contributions of the edge and basal plane etching using ReaxFF- based molecular dynamics (MD) and linking these processes together via a mechanistic model. The simulations were performed with the C++-based open source LAMMPS code.

## Results & Impact

Results demonstrate distinct ion energy regimes for isotropic versus anisotropic etching. These distinctive etching mechanisms, which are operative within narrow ion energy regimes, fully explain the differing plasma-graphene reactions observed experimentally.

## Why Blue Waters

The Blue Waters computational capacities were necessary for several reasons. First, the complex chemistry and plasma surface interactions involved in the hydrogen etching of graphene require the use of fully reactive MD potential, allowing for potential reactions between the Si, O, C, and H species at each MD time step. Second, the impact dynamics of impinging H atoms on graphene requires the use of a small time step (0.15 fs), which further increases computational cost. Third, studying the edges of the multilayer graphene presents a wide range of possible configurations, as the edges can be partially or completely covered by a graphene layer. Finally, because of the random process of H deposition, a large number of simulation runs are required to obtain statistically significant findings.