Holes in graphene and how to repair them

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Graphite is an important surface lining material for systems operating under high temperature and high pressure, and is being tested as surface material for rocket nozzles and for plasma divertors in nuclear fusion technology. Despite the importance of these technologies, very little is known about the high-temperature, high-pressure (high-T,P) processes causing graphite erosion due to reactions with oxidizing agents from fuel combustion, or the high-temperature chemical sputtering of hydrogen causing hydrocarbon yield at the plasma-wall interface in fusion reactors. It has become clear in numerous theoretical and experimental studies that existing holes in the basal graphite (0001) are premier places for attack of erosive species resulting in ever larger holes, and that therefore knowledge of the chemical stability of hole edges and techniques for "hole filling" are important to improve the performance of the graphitic wall material.

In this presentation we will present a) high-T quantum chemical molecular dynamics (QM/MD) guided reaction profile mapping for the annealing of a monovacancy defect in a small graphene flake, b) discuss the thermodynamic and kinetic stabilities of armchair and zigzag edges of large holes in graphite, and c) present high-T QM/MD simulations for hole-healing where holes in graphite are subjected to a vapor consisting of C_2 molecules (see Figure 1). We will briefly discuss our outlook on the future role of high-T QM/MD-guided global reaction route mapping (GRRM) for the presented simulations.

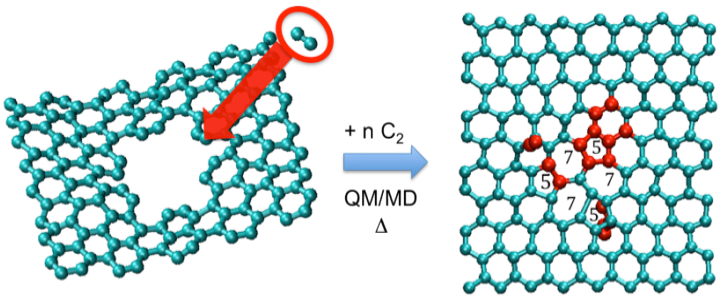

Figure 1. C_2 molecules used to gradually "fill" a hole in graphite in QM/MD simulations at 3000 K.