In this section, an exhaustive list of $x$, $y$, $z$ positions of carbon atoms for one selected simulation is enumerated.

Each simulation starts with a unit cell incorporating 2232 carbon atoms. The size of the $x$-$y$ plane of the unit cell is chosen such that the density of atoms is exactly equal to pristine graphene with periodic boundary condition (PBC), and the shape of the plane is nearly square, explicitly, 76.29Å×76.72Å. No PBC is imposed along $z$ direction. At the first step, 2232 carbon atoms are randomly put in the $x$-$y$ plane, with the constraint that the distance of any two atoms is no less than 1.2Å, to avoid unphysical states. Then a conjugate gradient (CG) method is performed to achieve a new configuration with force balance. The atoms of the obtained new configuration are still in the $x$-$y$ plane because none of the atoms feels a force along $z$ direction, therefore the CG method will cause no out-of-plane movements. Next, each atom is randomly moved along the $z$-direction by a distance from -0.1Å to +0.1Å, in order to let the configuration in the afterward simulation process have an out-of-plane degree of freedom under CG, hence the initial configuration is established.

Based on the initial configuration, a kinetic Monte Carlo (kMC) simulation is performed for $5\times10^5$ steps under fixed simulation temperature $T=6000K$. See also the flowchart in Fig 2 in the main body of the text.

II. List of Coordinates of Initial and Final Configurations

In this section, an exhaustive list of $x$, $y$, $z$ positions of carbon atoms for one selected individual simulation at the start and at the end is presented.

**Initial configuration**

**Supporting Information**

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