ReaxFF-nn: A Reactive Machine Learning Potential in GULP/LAMMPS and the Applications in the Thermal Conductivity Calculations of Carbon Nanostructures

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-Supporting Information-

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1. The convergence test of graphene sheet of potential ReaxFF-*nn*. The calculations show the value of κ is converged at Q-grid of *24×24×1*. The final value of κ is scaled by the diameter r_d of graphene sheet, i.e.:

$$\kappa = \kappa_{uncorrected}\frac{r_z}{r_d} \qquad \text{(s1)},$$

where $r_z = 10.0$ Å and $r_d = 3.35$ Å.

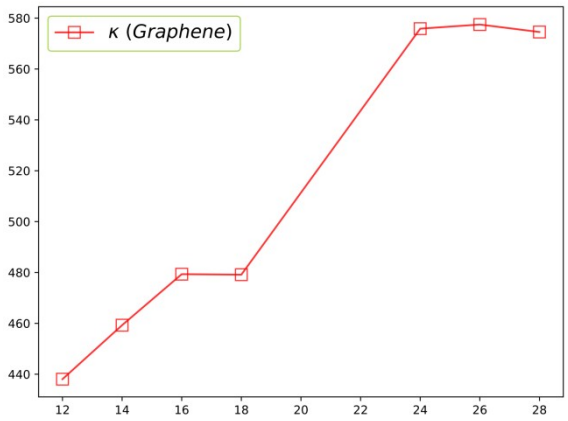

Figure S1. The unscale value of κ as a function of the value of Q-grid of graphene calculated by ReaxFF-*nn* potential.

2. The convergence test of graphene sheet of potential GAP-20. The calculations show the value of κ is converged at Q-grid of *28×28×1*. The value is corrected by eq. (s1).

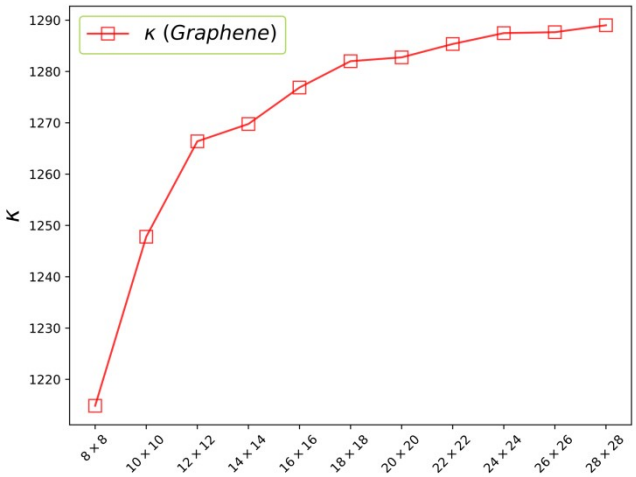

Figure S2. The unscale value of κ as a function of the value of Q-grid of graphene calculated by

GAP-20 potential.

3. The convergence test of CNT(5,5), CNT(6,6), CNT(7,7) and CNT(8,8) of potential ReaxFF-*nn*. The calculations show the value of κ is converged at Q-grid of *1×1×38*.

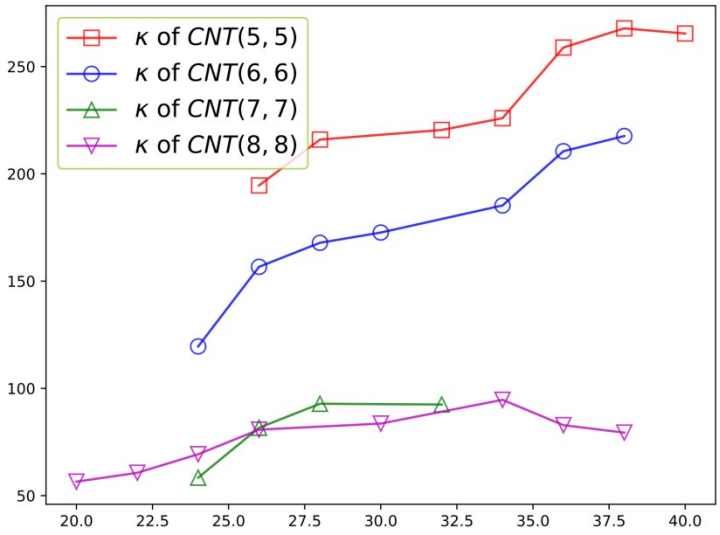

Figure S3. The value of κ as a function of the value of Q-grid of graphene calculated by ReaxFF-*nn* potential.

4. An oxygen molecule impacts the graphene surface at the A and B sites with initial velocities of 0.1, 0.15, 0.2, and 0.25 Å/fs along the Z axis. These simulations are conducted using ReaxFF-*nn* potential implemented in the LAMMPS package with parameters trained on the energies and forces of sample configurations by our 'I-ReaxFF' package.

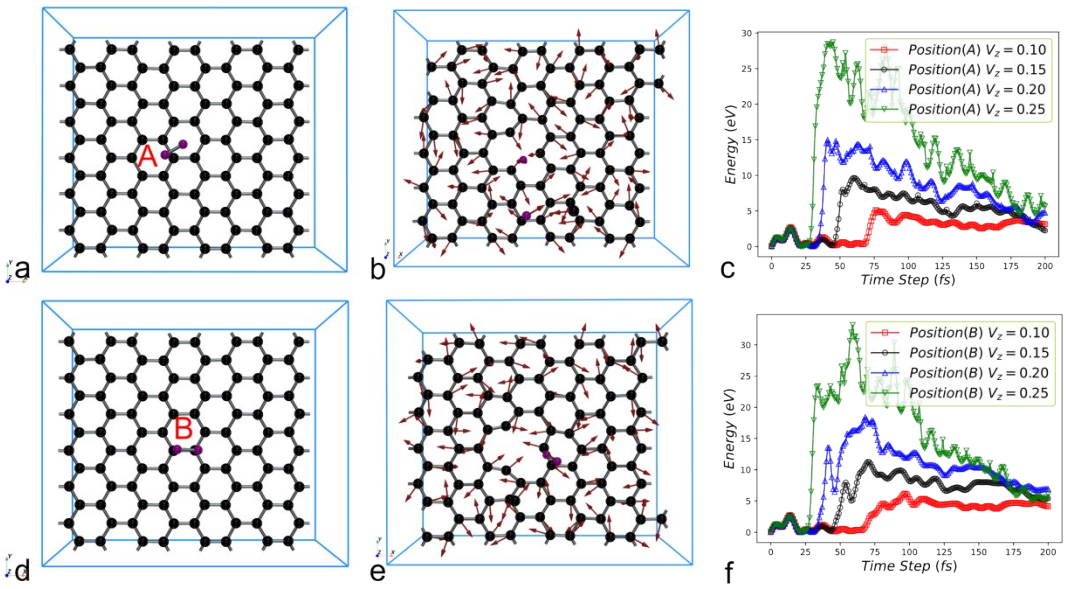

Figure S4. (a) The atomic configuration with oxygen at position A. (b) The final configuration after 200 fs MD simulations of position A, with oxygen molecule moving toward the graphene surface at a velocity 0.25 Å/fs. (c) The evolution of potential energy during MD simulations, with the oxygen molecule moving long the Z-axis at velocities ranging from 0.1 to 0.25 Å/fs and impacting at site A. (d) The atomic configuration with oxygen at position B. (e) The final configuration after 200 fs MD simulations of position B. (f) The evolution of potential energy during MD simulations, with oxygen molecule impact at site B.