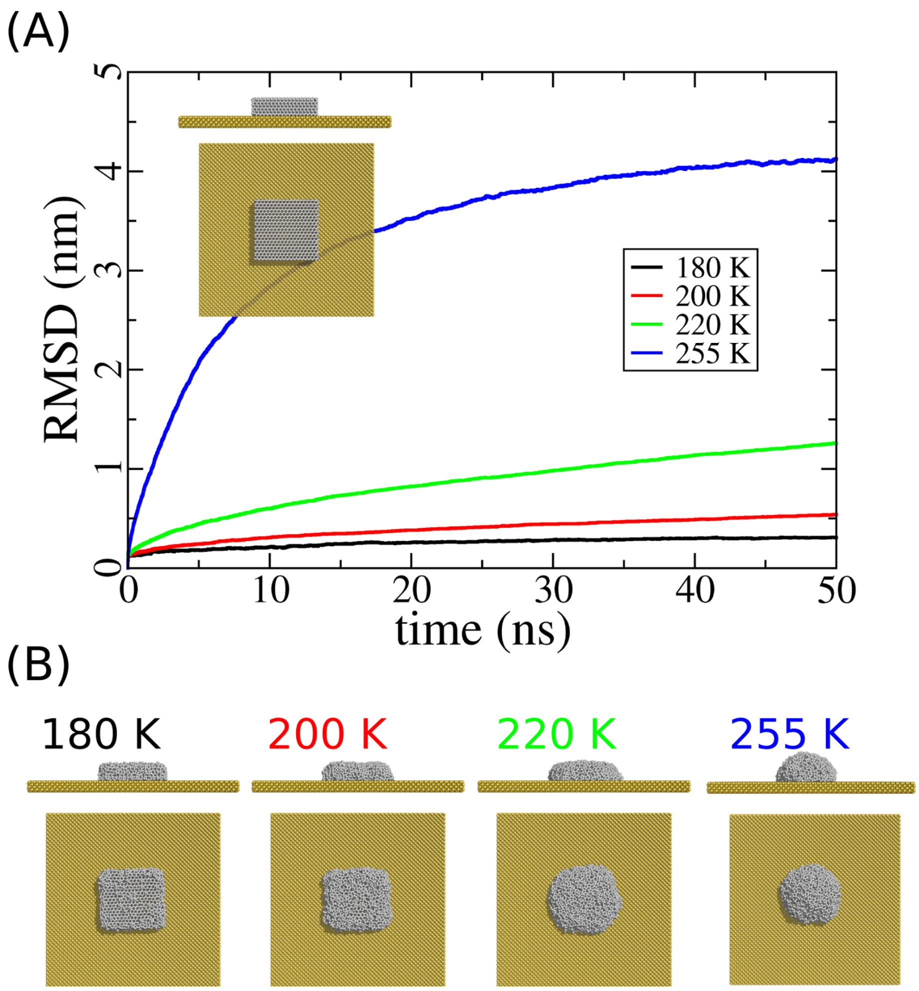
Supplementary Material

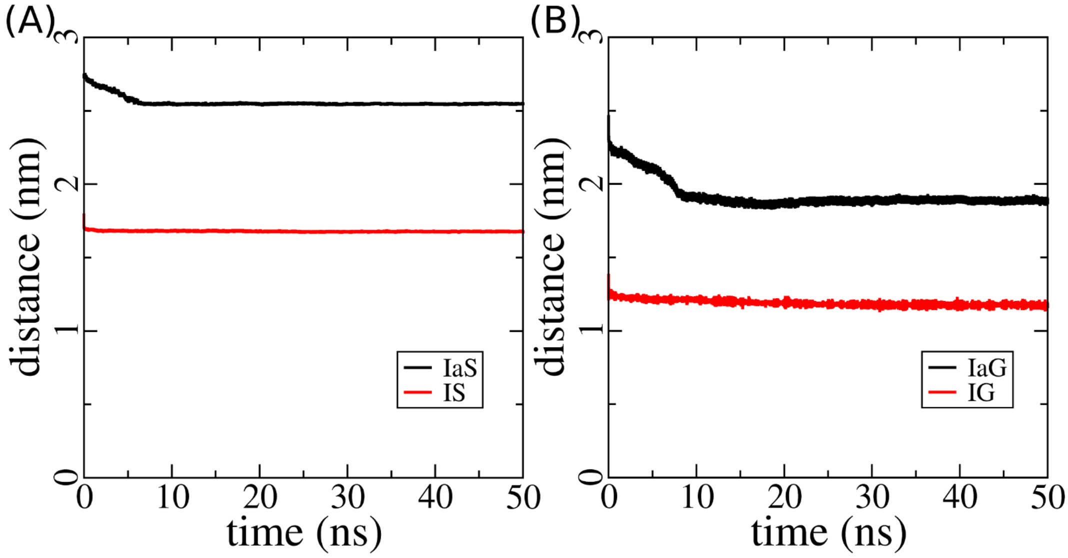
Supplementary movie

An example simulation movie file with ice detaching from graphene surface is given here. An aqueous water layer is sandwiched between the ice cube and the substrate in this simulation system.

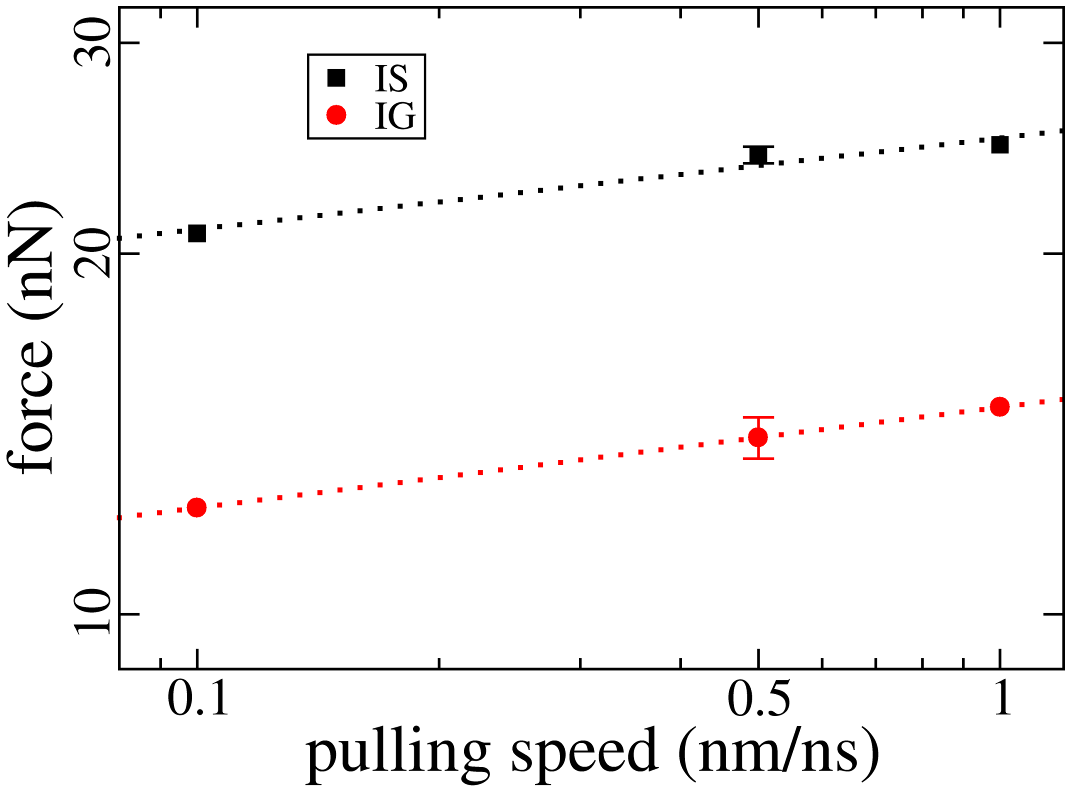
Supplementary Figures



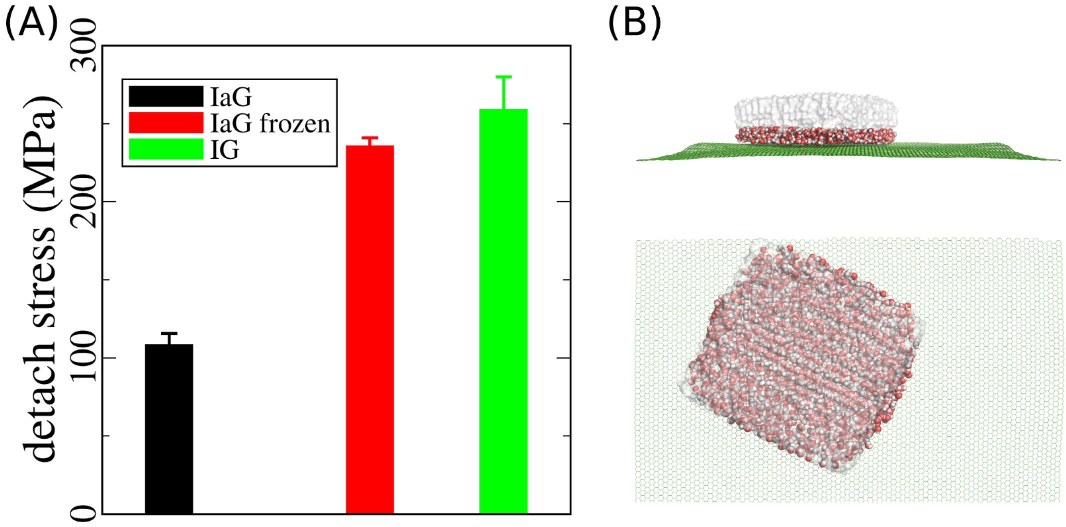
Supplementary Figure S1: **Nanoscale tip4p/ice ice cube stability at different temperatures.** (A) the root-mean-squared-deviation (RMSD) of the ice cube structures during equilibration at different temperatures ranging from 180 K to 255 K. The common initial structure for these simulations is shown as inset, both side view and top view, with the substrate in golden and the ice cube in gray. Different temperatures used in the simulations are shown as legend. (B) Final simulation snapshots at 50 ns. All the snapshots are shown with a sideview on top and a top view at the bottom.



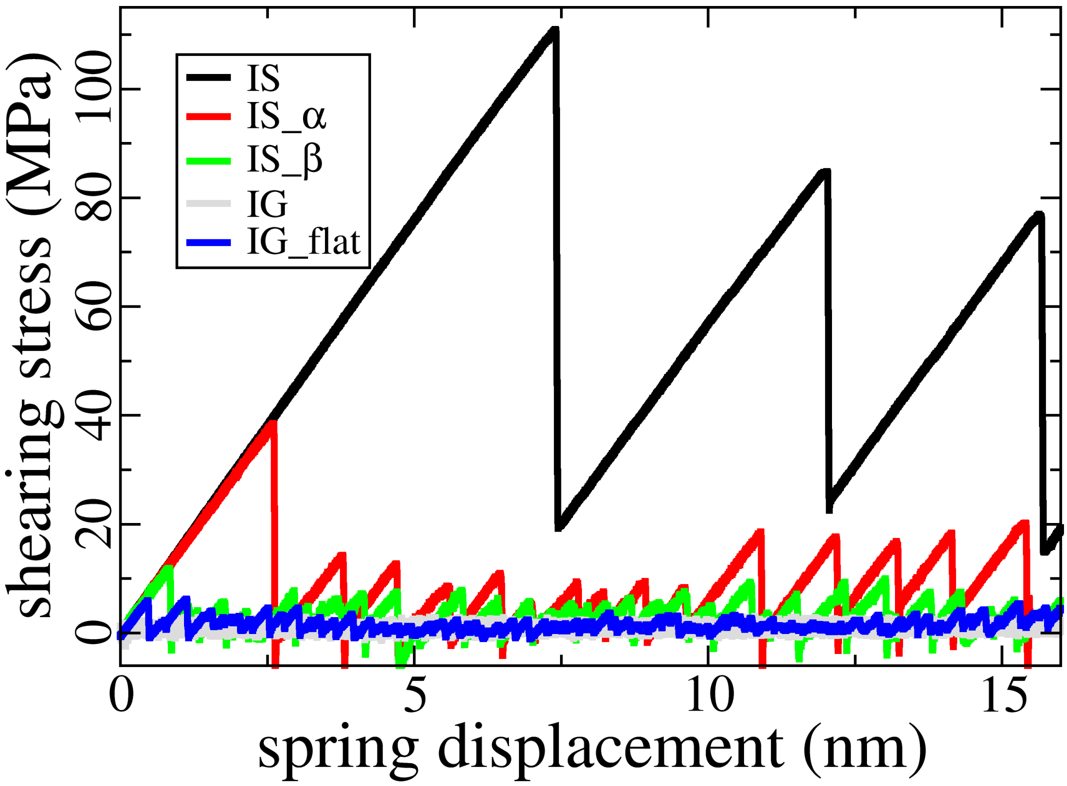
Supplementary Figure S2: **Distances between the center of mass of the ice cube and the substrates during equilibrating simulations.** (A) data from ice on silicon systems, with the black curve from the IaS system and the red curve from the IS system. (B) data from ice on graphene systems, with the black and red curves from the IaG and the IG system, respectively.



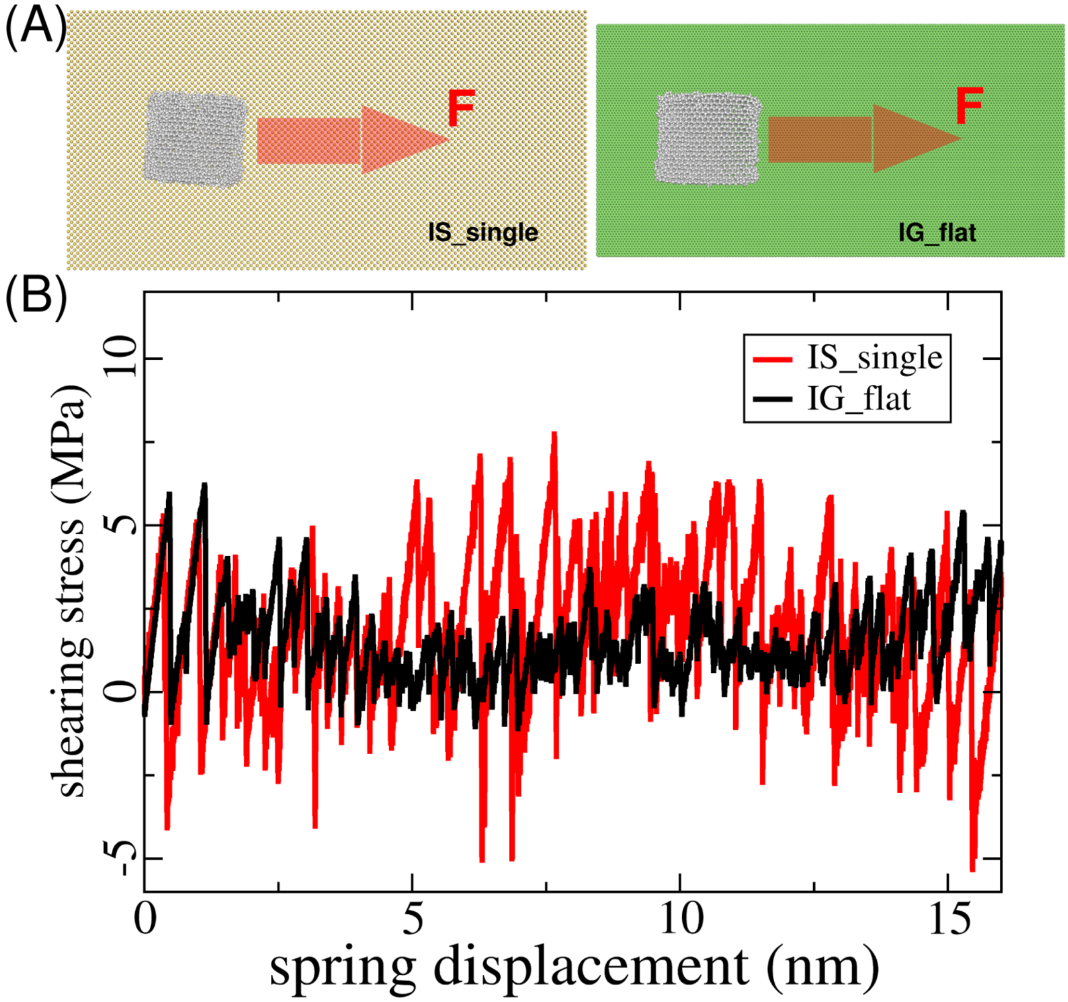
Supplementary Figure S3: **Loading rate denpendence of the ice detaching forces, exemplified by the IS and the IG systems.** Lower (0.1 nm/ns) and higher (1 nm/ns) pulling speeds are applied to the two systems, to compare with results obtained by using pulling speed of 0.5 nm/ns in the main text. Dashed lines are linear fitting in the log-log plot to show the increasing pattern of the rupture forces.



Supplementary Figure S4: **Detaching stress of the ice cube from graphene surface with crystallization of the aqueous water layer during the simulations.** (A) the detaching stress of the ice cube with crystallized aqueous layer is shown in red (IaG frozen). For comparison, detaching stress from the IaG system is shown in black, and detaching stress from the IG system is shown in green. (B) Simulation snapshot of the IaG frozen system with crystallized aqueous water layer. A sideview is on top, and a zoom-in top view is at the bottom. The ice cube is shown transparantly here for a better view on the crystallized water layer. Alignment of water molecules, and their forming of hexagonal molecular arrangement can be seen from the zoom-in top view.



Supplementary Figure S5: **Shearing stresses on surfaces with varied interfacial energy.** In order to clarify the interfacial energy effect on the shearing stress, the energy well depth (ϵ) of the silicon atoms in the IS system is first artificially reduced from 2.44704 kJ/mol/nm^2 to be the same with the carbon atoms in the IG system (0.29288 kJ/mol/nm^2). The shearing stress obtained in this new system, termed IS_α, is shown in red and has a mean value of 8.09$\pm$7.44 MPa. Given there are multilayer of atoms in the IS_α system, the interfacial energy is still much higher than the single atom layer of graphene. The silicon atom ϵ value is further reduced to 1/5 of the carbon atoms, namely 0.058576 kJ/mol/nm^2, to create another artificial system termed as IS_β. Shearing stress in the IS_β is shown in green, which has a mean value of 3.10$\pm$2.61 MPa. One other shearing test with the graphene in the IG system in constraint as a flat plane without any thermal fluctuation, termed as IG_flat system, is also performed. The shearing stress (blue curve) shows a saw-tooth pattern, and has a mean value of 1.58$\pm$1.22 MPa. Shear stresses observed in IS (black curve) and IG (gray curve) systems (Fig. 4 in the main text) are shown here for comparison.



Supplementary Figure S6: **Shearing ice cube on a single-layer silicon surface and on graphene.** (A) simulation systems for shearing the ice cube on single-layer silicon surface (left, termed **IS_single**) and on graphene (**IG_flat**, Suppl.Fig. S5). The silicon atoms are shown in gold, and the graphene is shown in green. Red arrows are used to indicate the shearing direction. (B) shearing stress profiles from the two systems, with mean value and standard deviation of 1.87±2.11 MPa and 1.58±1.22 MPa for **IS_single** and **IG_flat** respectively.