

File name: Supplementary Movie 1

Description: An MLFF MD simulation of spontaneous formation of the hexagonal monolayer ice from the 2D water.

File name: Supplementary Movie 2

Description: An MLFF MD simulation of spontaneous formation of the pentagonal monolayer ice from the 2D water.

File name: Supplementary Movie 3

Description: An MLFF MD simulation of spontaneous formation of the square monolayer ice by MLFF MD simulations.

File name: Supplementary Movie 4

Description: An MLFF MD simulation of spontaneous formation of the ZZMI monolayer ice by MLFF MD simulations.

File name: Supplementary Movie 5

Description: An MLFF MD simulation of spontaneous hexagonal-to-pentagonal transition.

File name: Supplementary Movie 6

Description: An MLFF MD simulation of spontaneous pentagonal-to-square transition.

File name: Supplementary Movie 7

Description: An MLFF MD simulation of spontaneous square-to-ZZMI transition.

File name: Supplementary Movie 8

Description: An MLFF MD simulation of spontaneous square-to-pentagonal transition.

File name: Supplementary Movie 9

Description: An MLFF MD simulation of phase transition from the 2D water to a final ZZ-qBI at 300 K with lateral pressure increasing from 0 to 20 GPa.

File name: Supplementary Movie 10

Description: An MLFF MD simulation of branched ZZ-qBI at constant lateral pressure of 15 GPa with temperature increasing from 10 K to 300 K.

File name: Supplementary Movie 11

Description: A 27-ps AIMD simulation of a ZZ-qBI ice at 20 GPa and 300 K.

File name: Supplementary Movie 12

Description: A 35-ps AIMD simulation of a bZZ-qBI ice at 15 GPa and 300 K.

File name: Supplementary Movie 13

Description: A 21-ps rev-PBE0-D3 AIMD simulation of a ZZ-qBI ice at 20 GPa and 300 K.

File name: Supplementary Movie 14

Description: A 26-ps rev-PBE0-D3 AIMD simulation of a bZZ-qBI ice at 15 GPa and 300 K.

File name: Supplementary Movie 15

Description: A 27-ps AIMD simulation of a ZZ-qBI ice at 300 K with real graphene walls.

File name: Supplementary Movie 16

Description: A 23-ps AIMD simulation of a bZZ-qBI ice at 300 K with real graphene walls.

File name: Supplementary Movie 17

Description: A 20-ps AIMD simulation of a ZZ-qBI ice at 350 K with real graphene walls.

File name: Supplementary Movie 18

Description: A 20-ps AIMD simulation of a bZZ-qBI ice at 350 K with real graphene walls.

File name: Supplementary Movie 19

Description: A 20-ps BLYP-D3 AIMD simulation of a ZZ-qBI ice at 350 K with real graphene walls.

File name: Supplementary Movie 20

Description: A 20-ps BLYP-D3 AIMD simulation of a bZZ-qBI ice at 350 K with real graphene walls.

File name: Supplementary Movie 21

Description: A 11-ps revPBE0-D3 AIMD simulation of a ZZ-qBI ice at 350 K with real graphene walls.

File name: Supplementary Movie 22

Description: A 1-ns PIMD simulation of a ZZ-qBI ice at 300 K, using a timestep of 0.25 fs.

File name: Supplementary Movie 23

Description: A 1-ns PIMD simulation of a bZZ-qBI ice at 300 K, using a timestep of 0.25 fs.

File name: Supplementary Movie 24

Description: A 1-ns MLFF MD simulation of ZZ-qBI at 300 K and 8-10 GPa within a nanoslit of 6.5 Å width, using a timestep of 0.2 fs.

File name: Supplementary Movie 25

Description: A 1-ns MLFF MD simulation of bZZ-qBI at 300 K and 10-15 GPa within a nanoslit of 6.5 Å width, using a timestep of 0.2 fs.

File name: Supplementary Movie 26

Description: A 1-ns MLFF MD simulation of ZZ-qBI at 300 K and >50 GPa within a nanoslit of 5.5 Å width, using a timestep of 0.2 fs.

File name: Supplementary Movie 27

Description: A 1-ns MLFF MD simulation of bZZ-qBI at 300 K and >50 GPa within a nanoslit of 5.5 Å width, using a timestep of 0.2 fs.

File name: Supplementary Movie 28

Description: A 1-ns PIMD simulation of transformation of qBI to ZZMI at 300 K within a nanoslit of 5.0 Å width, using a timestep of 0.25 fs.

File name: Supplementary Movie 29

Description: A 26-ps AIMD simulation of a hexagonal ice at 0.025 GPa and 150 K.

File name: Supplementary Movie 30

Description: A 20-ps AIMD simulation of a pentagonal ice at 0.25 GPa and 150 K with real graphene walls.

File name: Supplementary Movie 31

Description: A 26-ps AIMD simulation of a square ice at 2.5 GPa and 200 K.

File name: Supplementary Movie 32

Description: A 26-ps AIMD simulation of a ZZMI ice at 10.0 GPa and 300 K.

File name: Supplementary Movie 33

Description: A 21-ps AIMD simulation of the LD-48MI at -0.4 GPa and 50 K with real graphene walls.

File name: Supplementary Movie 34

Description: A 2.9-ps AIMD simulation of spontaneous LD-48MI-to-gas transition at -0.5 GPa and 100 K.

File name: Supplementary Movie 35

Description: A 11.1-ps AIMD simulation of spontaneous LD-48MI-to-gas transition at -0.3 GPa and 150 K.

File name: Supplementary Movie 36

Description: A 3.4-ps AIMD simulation of spontaneous hexagonal-to-gas transition at -0.25 GPa and 180 K.