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# SUPPORTING INFORMATION FOR

## Mechanical Properties of Amorphous $CO_2$ Hydrates: Insights from Molecular Simulations

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**Figure S1**

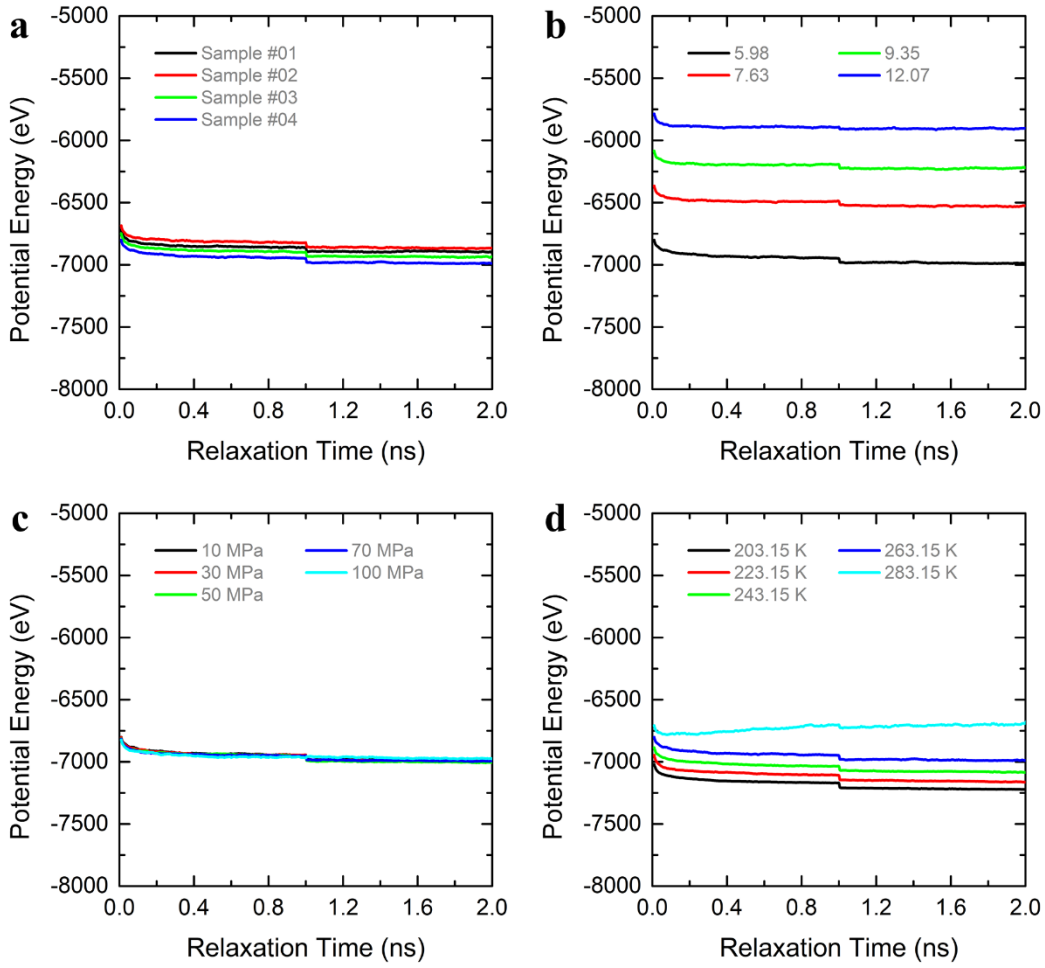


**Figure S1. Potential energy of amorphous $CO_2$ hydrates.** (a) Four amorphous $CO_2$ hydrate systems with a water/$CO_2$ ratio of about 5.98 at 263.15 K and 100 atm. (b) Different water/$CO_2$ ratios at 263.15 K and 100 atm. (c) Different confining pressures with a water/$CO_2$ ratio of about 5.98 at 263.15 K. (d) Different temperatures with a water/$CO_2$ ratio of about 5.98 at 100 atm.

**Figure S2**

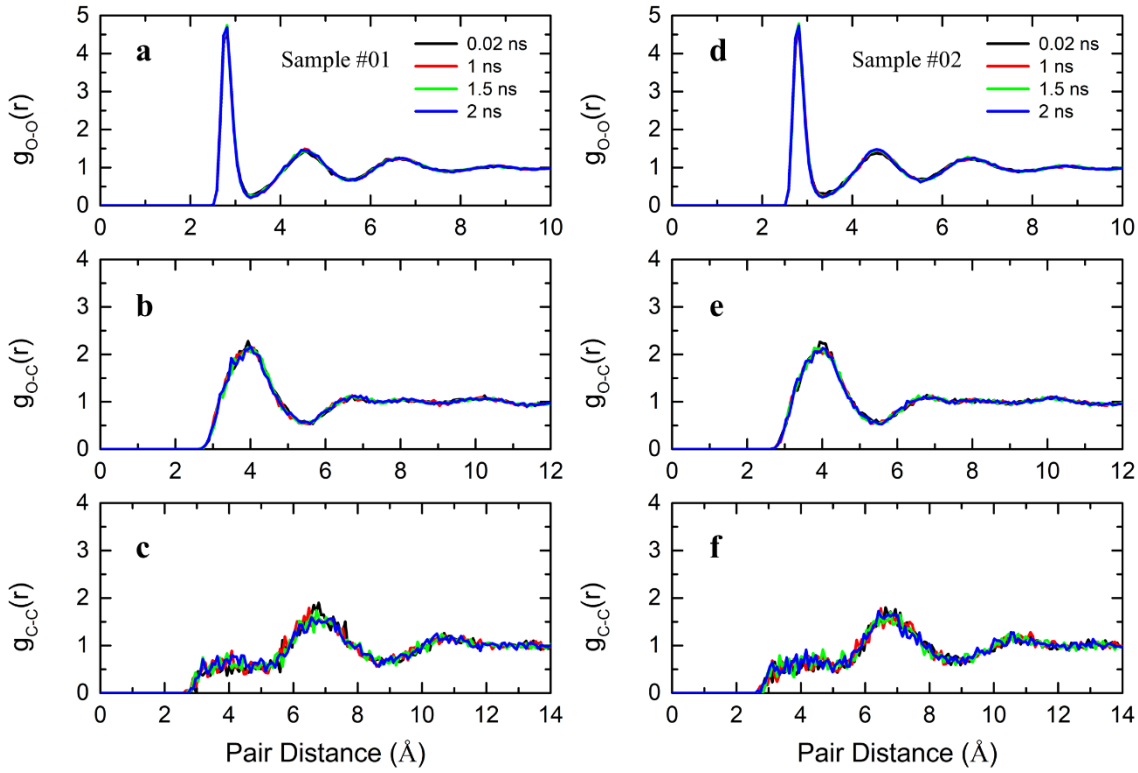


**Figure S2. Radial distribution function (RDF) of amorphous $CO_2$ hydrates with a water/$CO_2$ ratio of about 5.98 at 263.15 K and 100 atm.** (a)-(c) Sample #01 of the six prepared samples at different relaxation states. (d)-(f) Sample #02 of the six prepared samples at different relaxation states.

**Figure S3**

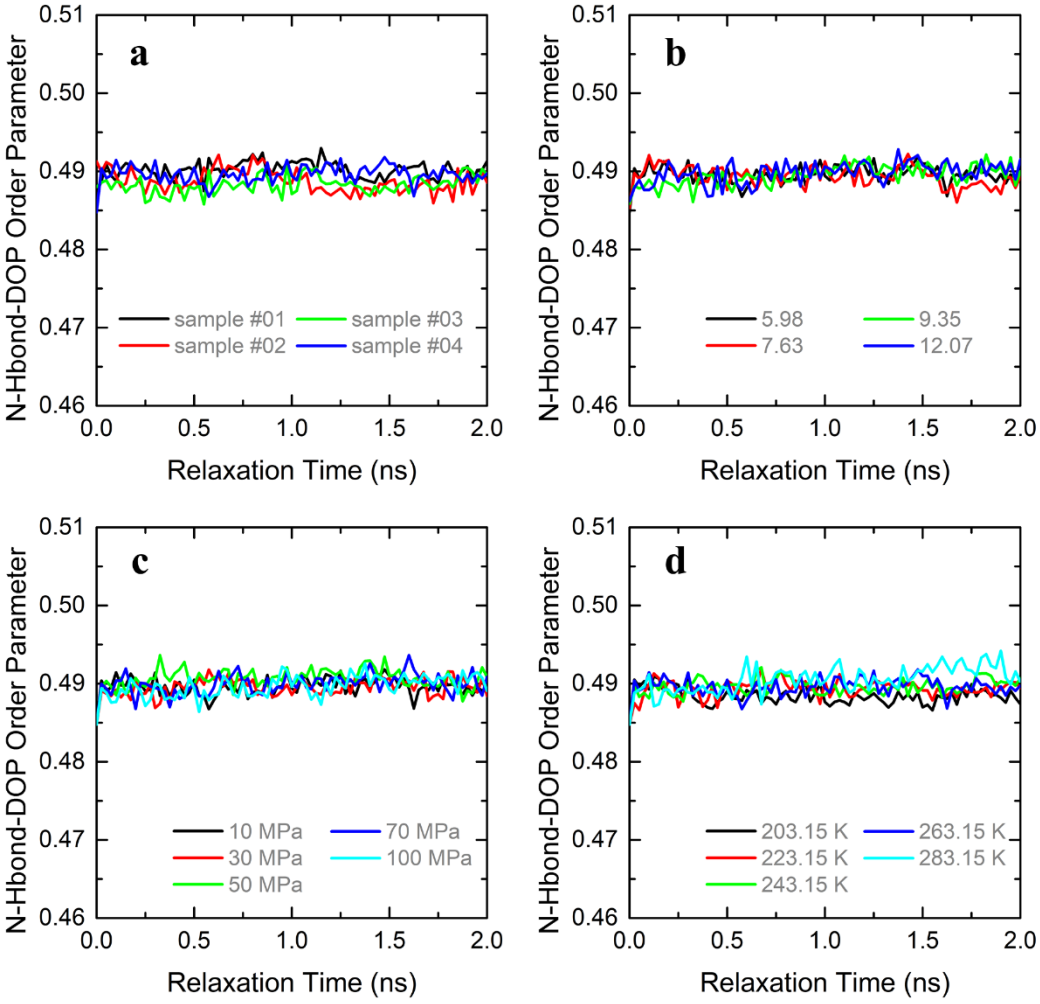


**Figure S3. N-Hbond-DOP order parameter of amorphous $CO_2$ hydrates.** (a) Different samples with a water/$CO_2$ ratio of about 5.98 at 263.15 K and 100 atm. (b) Different water/ $CO_2$ ratios at 263.15 K and 100 atm. (c) Different confining pressures with a water/$CO_2$ ratio of about 5.98 at 263.15 K. (d) Different temperatures with a water/$CO_2$ ratio of about 5.98 at 100 atm.

**Figure S4**

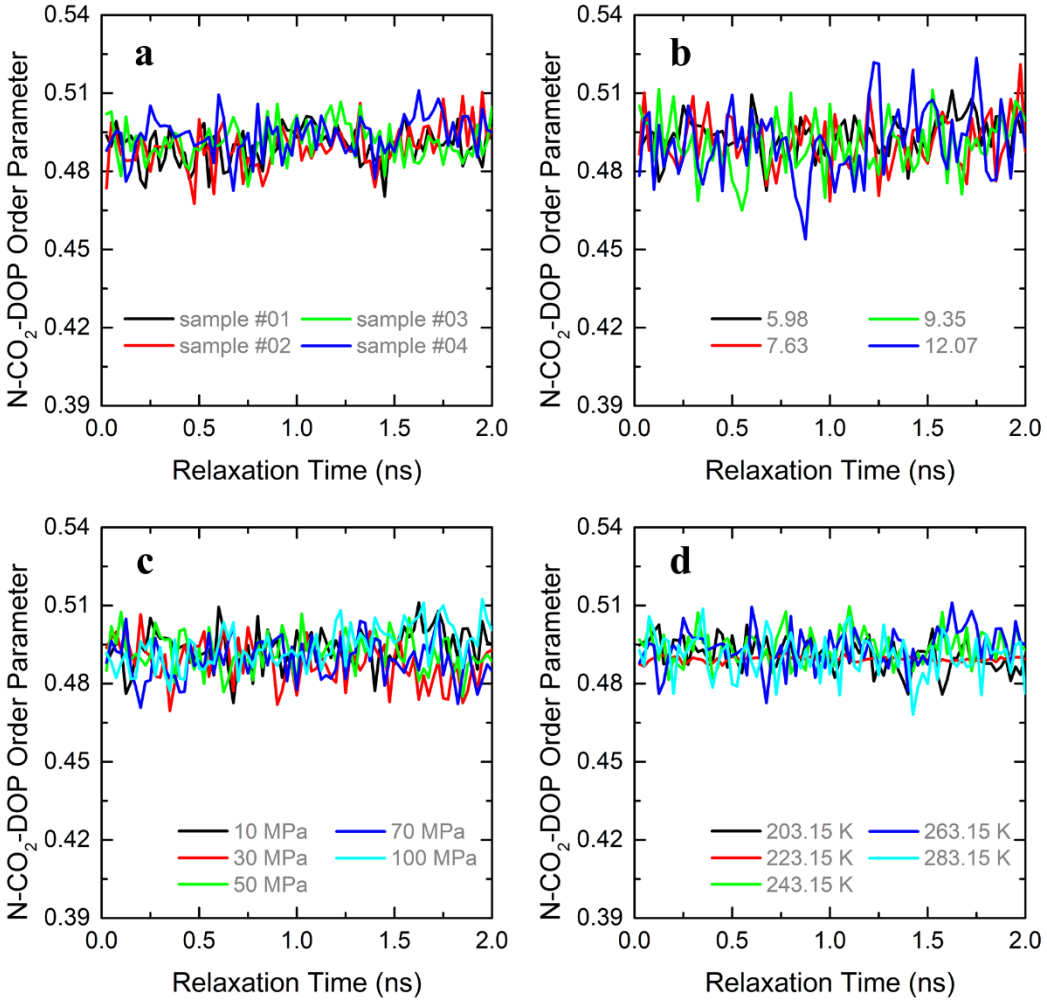


**Figure S4. N-$CO_2$-DOP order parameter of amorphous $CO_2$ hydrates.** (a) Different samples with a water/$CO_2$ ratio of about 5.98 at 263.15 K and 100 atm. (b) Different water/ $CO_2$ ratios at 263.15 K and 100 atm. (c) Different confining pressures with a water/$CO_2$ ratio of about 5.98 at 263.15 K. (d) Different temperatures with a water/$CO_2$ ratio of about 5.98 at 100 atm.

**Figure S5**

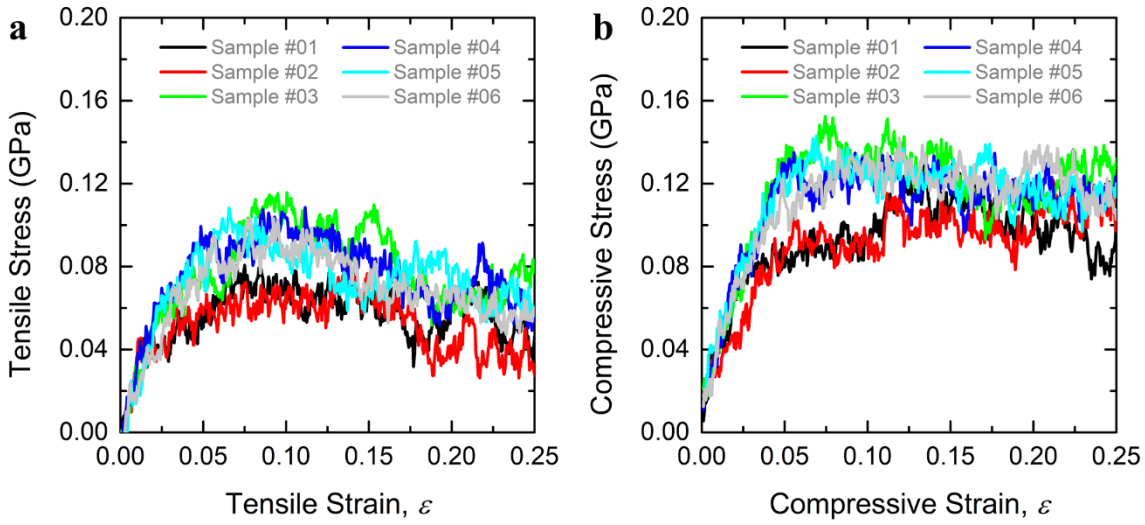


**Figure S5. Mechanical properties of six different amorphous $CO_2$ hydrate samples with a water/$CO_2$ ratio of about 5.98 at 263.15 K and 100 atm.** (a) Tension loads. (b) Compression loads.

**Figure S6**

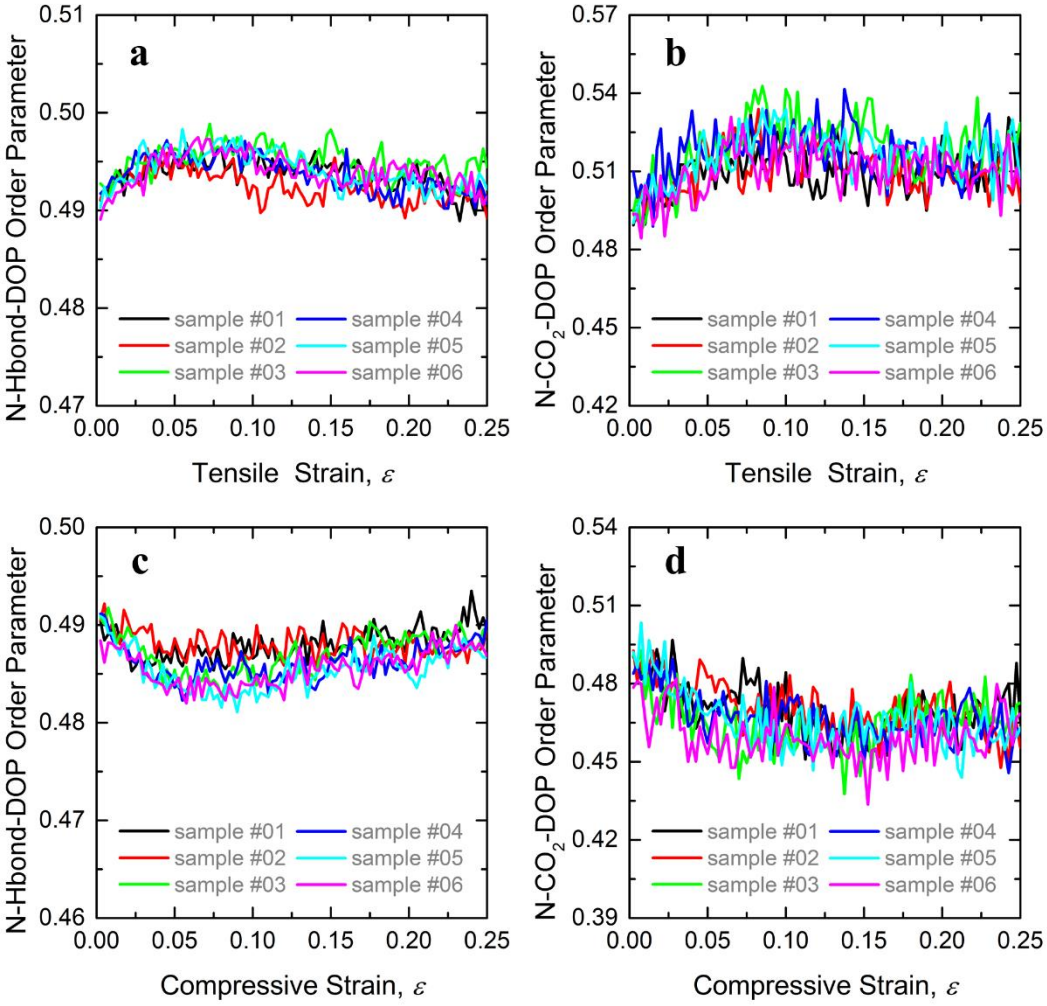


**Figure S6. DOP order parameter of amorphous $CO_2$ hydrates with a water/$CO_2$ ratio of about 5.98 at 263.15 K and 100 atm.** (a) N-Hbond-DOP order parameter under tension. (b) N-$CO_2$-DOP order parameter under tension. (c) N-Hbond-DOP order parameter under compression. (d) N-$CO_2$-DOP order parameter under compression.

**Figure S7**

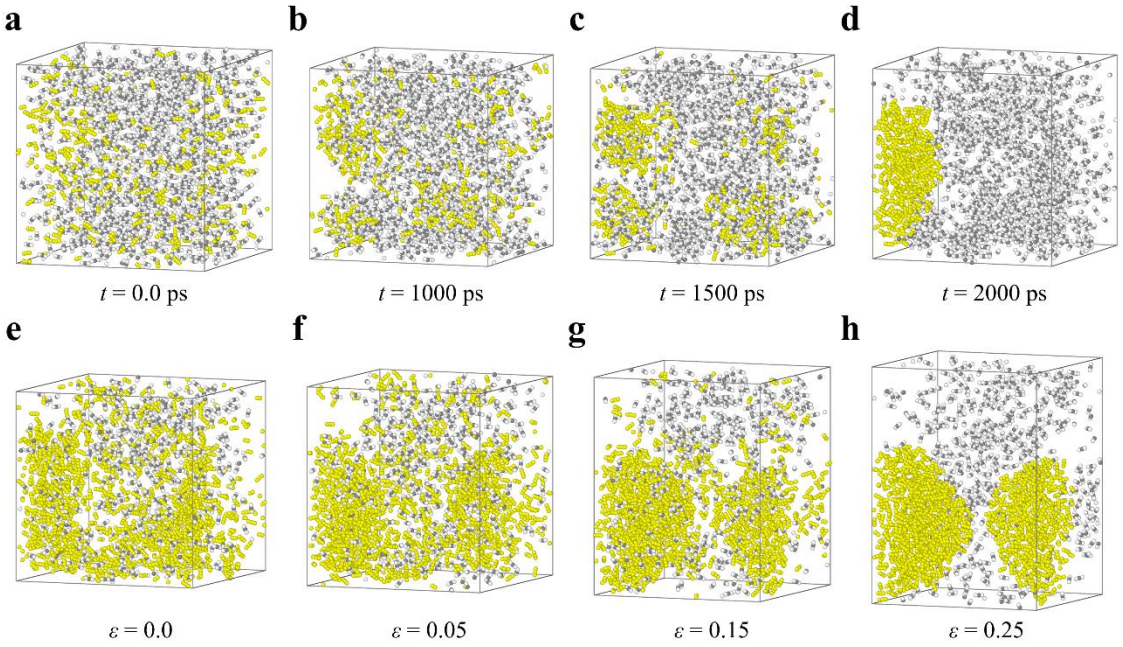


**Figure S7. Molecular structures of $CO_2$ molecules in amorphous $CO_2$ hydrates with a water/$CO_2$ ratio of about 5.98 at 283.15 K and 100 atm.** (a)-(d) Perspective views of $CO_2$ molecules in amorphous $CO_2$ hydrates at different relaxation times. (e)-(h) Perspective views of $CO_2$ molecules in amorphous $CO_2$ hydrates at different tensile strains. In Figure S7, some $CO_2$ molecules are rendered by yellow to monitor the formation of $CO_2$ nanobubble.

**Movies S1-S3**

Movies S1-S3. Visualization of amorphous $CO_2$ hydrates under tension. S1: A sample with a water/$CO_2$ ratio of 12.07 at 263.15 K and 100 atm. S2: A sample with a water/$CO_2$ ratio of 5.98 at 263.15 K and 700 atm. S3: A sample with a water/$CO_2$ ratio of 5.98 at 203.15 K and 100 atm. All water structures are colored by the potential energy. Carbon and Oxygen atoms in $CO_2$ molecules are colored with grey and white, respectively. Hydrogen atoms in water molecules are not shown for clarity.

**Movies S4-S6**

Movies S4-S6. Visualization of amorphous $CO_2$ hydrates under compression. S1: A sample with a water/$CO_2$ ratio of 12.07 at 263.15 K and 100 atm. S2: A sample with a water/$CO_2$ ratio of 5.98 at 263.15 K and 700 atm. S3: A sample with a water/$CO_2$ ratio of 5.98 at 203.15 K and 100 atm. All water structures are colored by the potential energy. Carbon and Oxygen atoms in $CO_2$ molecules are colored with grey and white, respectively. Hydrogen atoms in water molecules are not shown for clarity.

**Movies S7-S8**

Movies S7-S8. Visualization of $CO_2$ molecules in amorphous $CO_2$ hydrates with a water/$CO_2$ ratio of 5.98 at 283.15 K and 100 atm. S7: A sample at relaxation process. S8: A sample under tension loads. Carbon and Oxygen atoms in $CO_2$ molecules are colored with grey and white, respectively. Water molecules are not shown for clarity. In Movies S7-S8, some $CO_2$ molecules are rendered by yellow to monitor the formation of $CO_2$ nanobubble.