Supporting information

Ice Carbons

Hui-Yan Zhao, [1,2] Jing Wang,[1,3] Xiu-Jie Su,[1,3] Dong-Bo Zhang,[2] and Ying Liu[1,3,*]

[1]*Department of Physics and Hebei Advanced Thin Film Laboratory, Hebei Normal University, Shijiazhuang 050024, China.*

[2]*Beijing Computational Science Research Center, Beijing 100084, China*

[3]*National Key Laboratory for Materials Simulation and Design, Beijing 100083, China.*

Figure S1 shows the probability distributions of atomic displacements with respect to the ice-carbon structures shown in Fig. 1 at about 250 K. As shown in Fig. S1, bell-shaped distribution curves centered at zero displacements are found in the three Cartesian directions. The probability distribution of atomic displacements is maximal at the equilibrium position around which the atom oscillates, indicating that the equilibrium structures of these ice-carbon structures are the ones shown in Fig. 1.

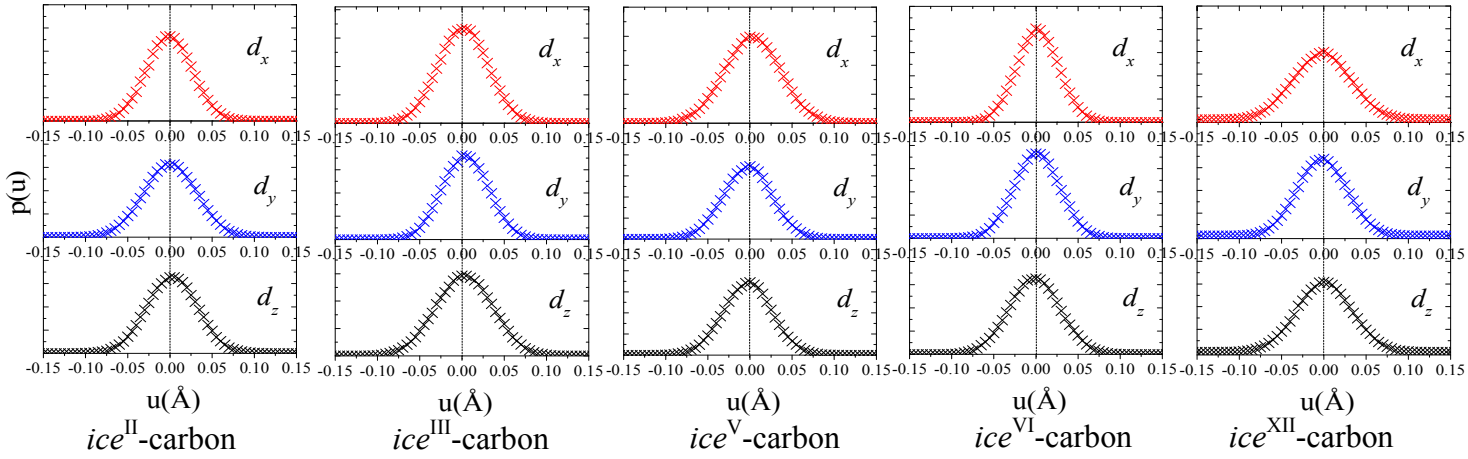

Figure S1 (color online). Probability distributions of atomic displacements with respect to the ice-carbon structures shown in Fig. 1 at about 250 K.

* Correspondence author. E-mail: yliu@hebtu.edu.cn