

Supplementary Information for “nanostructured water and Carbon dioxide inside collaping carbon nanotbes at high pressure”

Wenwen Cui,^a Tiago F.T. Cerqueira,^{b,a} Silvana Botti,^{b,a,c} Miguel A.L. Marques,^{*d,a,c} and Alfonso San-Miguel^a

^a*Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon, F-69622 Villeurbanne Cedex, France*

^b*Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany*

^c*European Theoretical Spectroscopy Facility*

^d*Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany*

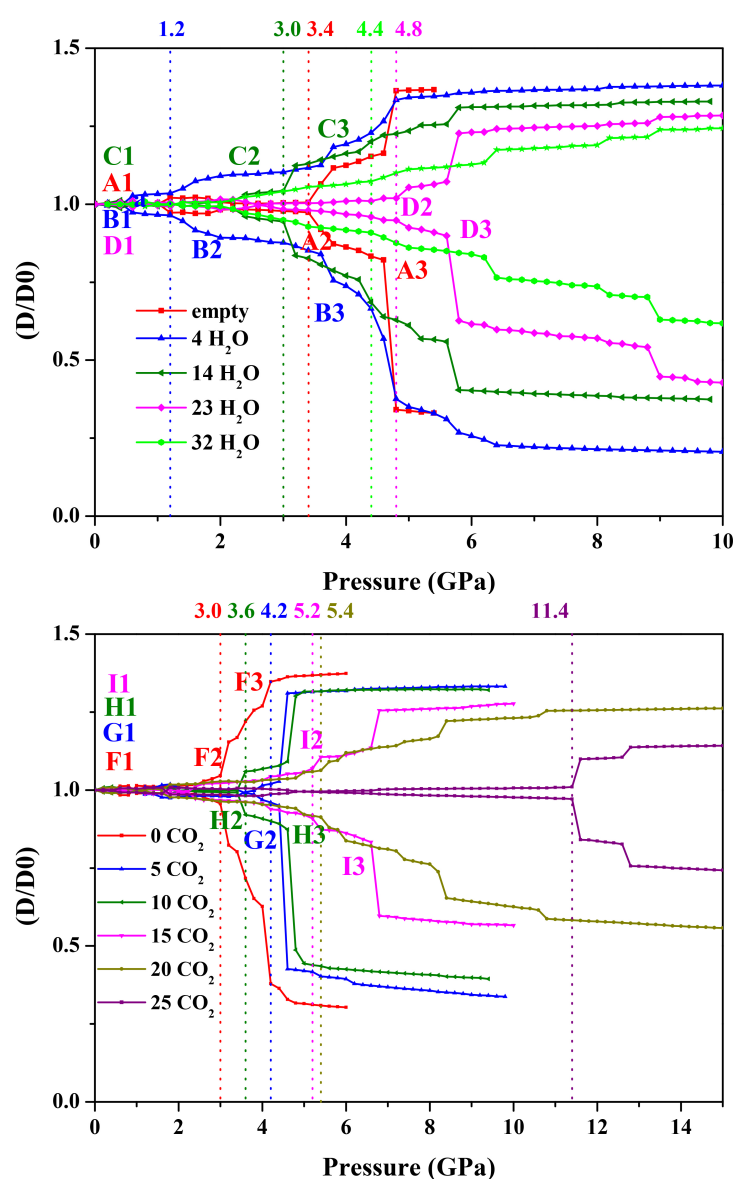


Fig. S1. Variation of distance from two pairs of C atoms belonging to the (10,10) CNTs filled with different amount of H_2O (upper panel) and CO_2 (lower panel) molecules as a function of pressure. The

segments formed by the pairs of C atoms are approximately perpendicular and their length is approximately equal to the tube diameter. The numbers indicate the onset pressure for the tube deformation P_o .

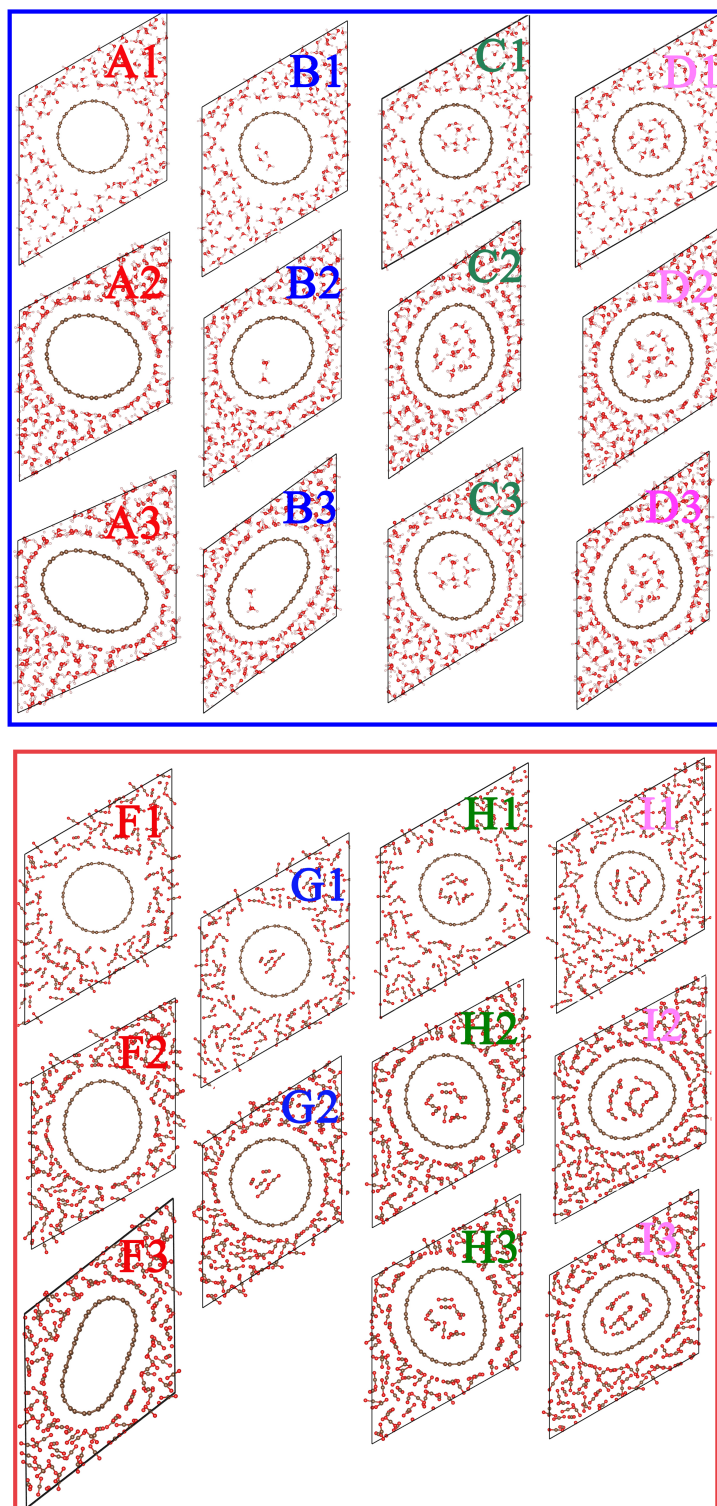


Fig. S2. CNTs structures for filling with different amounts of H_2O (upper panel) and CO_2 (lower panel) molecules, as in Fig. S1, before reaching the collapse pressure P_c