Abstract Submitted
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Modeling of the amorphous phase of poly-CO I.G. BATYREV, US Army Research Laboratory — We studied theoretically the details of amorphous structure of extended CO solid obtained by isotropic compression of solid CO phases in the range of 3-25 GPa. We performed DFT simulations of 128, 432, and 1024 atom models. Structures of random networks found at zero temperature were used for equilibration at finite temperatures up to 50 ps by employing first principles MD. We found that the polymerization begins at 6 - 8 GPa and a random network of 4-7 atom rings obtained above 15 GPa could exist up to 0.1 -0.25 GPa. We studied pressure induced changes in topological characteristic of the random network based on the rings statistics, radial distribution function and average number of the nearest neighbors (NN). NN found to be 3.2 for C and 1.7 for O for 128 atom system at 15 GPa. We performed vibration analysis of the systems as a function of pressure and calculated in dipole approximation IR intensity with identification of contributions from several main motifs of the amorphous structure. To understand charge distribution and localization and to find the possible "weakest link" in the network we calculated electron localization function for the most common fragments of amorphous poly-CO structure.

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