

Supplementary Materials for

Facile diamond synthesis from lower diamondoids

Sulgiye Park, Iwnetim I. Abate, Jin Liu, Chenxu Wang, Jeremy E. P. Dahl, Robert M. K. Carlson, Liuxiang Yang, Vitali B. Prakapenka, Eran Greenberg, Thomas P. Devereaux, Chunjing Jia, Rodney C. Ewing, Wendy L. Mao, Yu Lin*

*Corresponding author. Email: lyforest@stanford.edu

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Fig. S7. Representative Raman spectra of quenched samples after laser-heating octadecane at the synthesis pressure of 12.5 GPa.

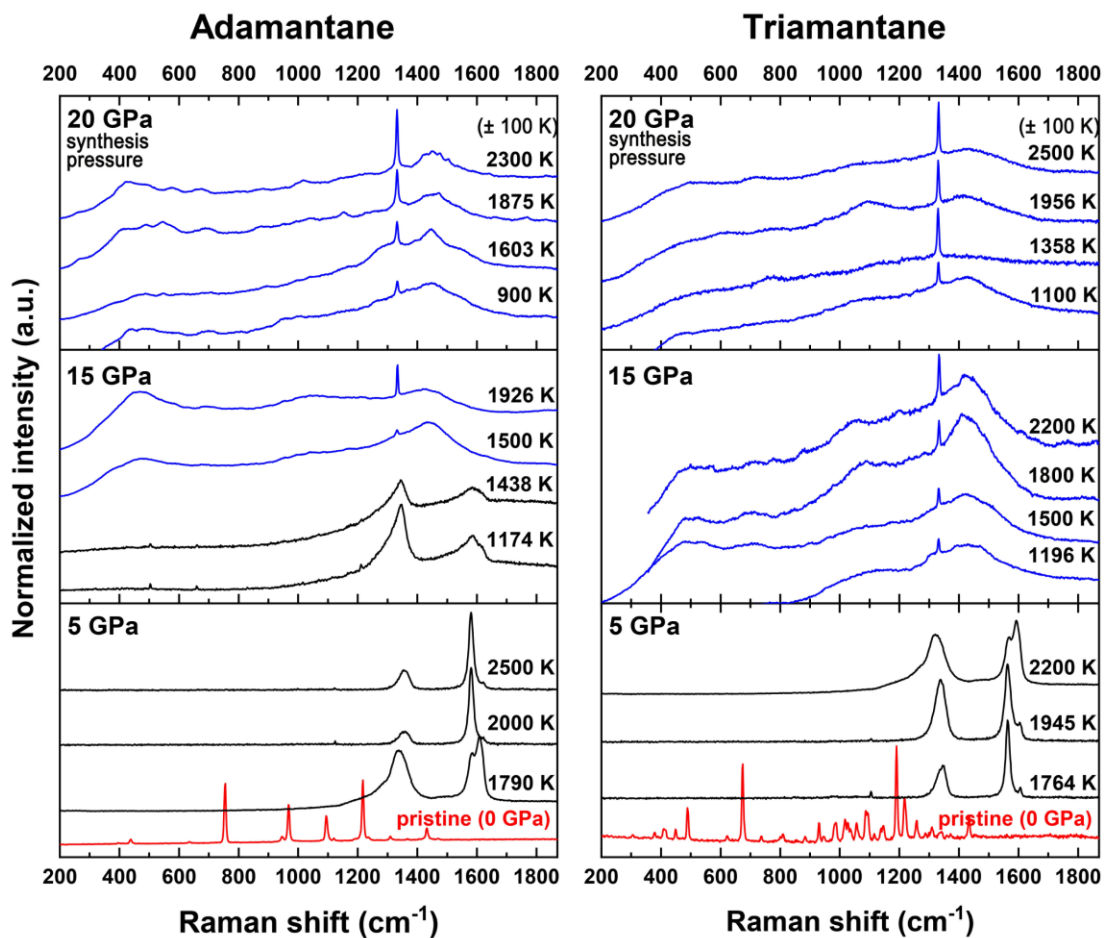


Fig. S1. Representative Raman spectra of quenched products after laser-heating adamantane and triamantane at pressures of 5, 15, and 20 GPa. Each Raman spectrum is collected from an individual laser-spot with a specific P - T value. All Raman measurements were collected after the samples had been quenched and removed from the diamond anvil cells.

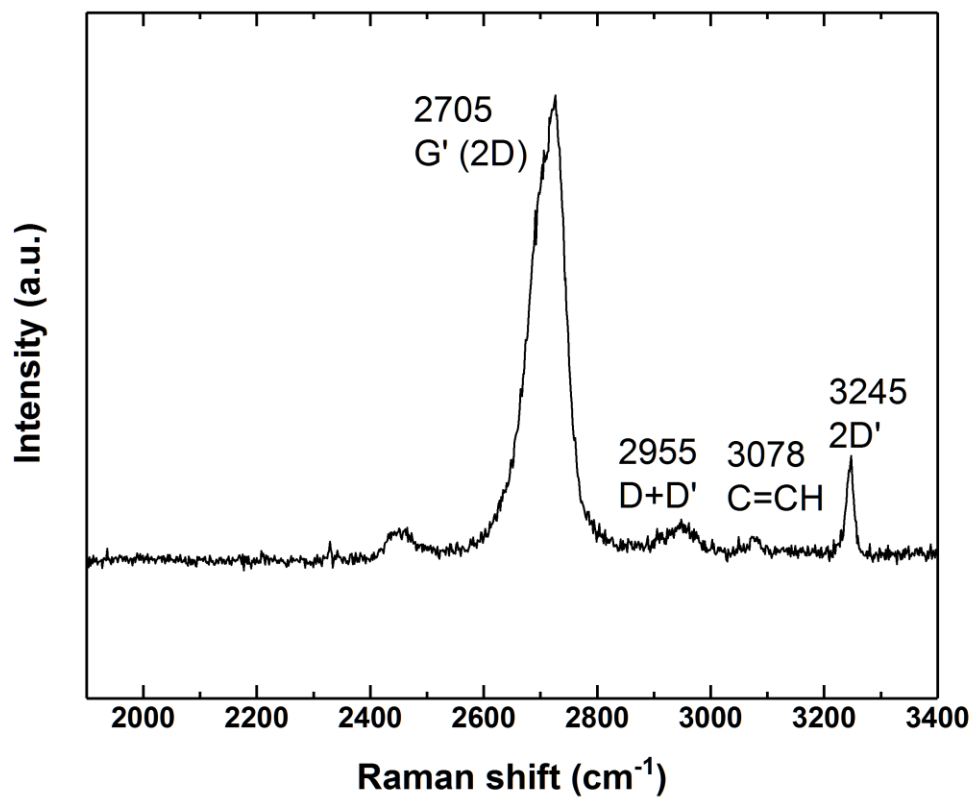


Fig. S2. Higher Raman frequency of adamantane compressed and heated to 10 GPa and ~2000 K. The spectrum was collected after the sample had been removed from the diamond anvil cell.

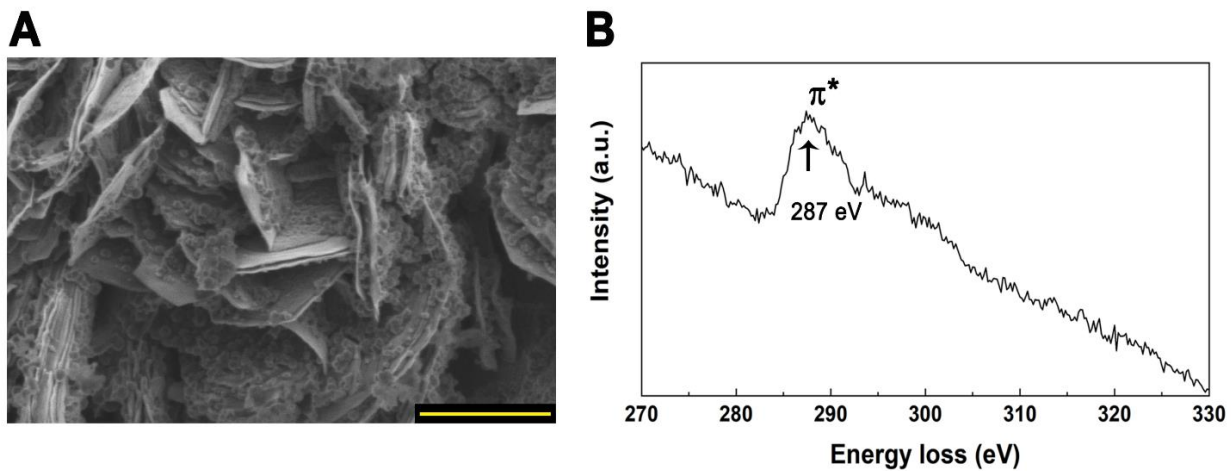


Fig. S3. Characterization of graphite formed from diamondoids. (A) A representative SEM image of graphite flakes formed from diamondoids. Scale bar is 2 μm . (B) EELS from a graphite flake represents a full sp^2 hybridization.

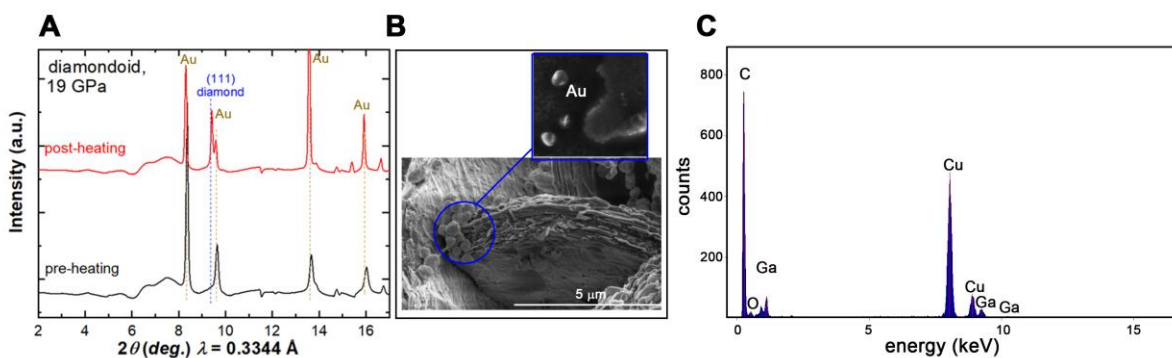


Fig. S4. XRD and SEM data of gold nanoparticles and energy-dispersive x-ray spectrum of diamond. (A) *In situ* XRD patterns of the starting and final product. Au signal is observed in the XRD patterns pre-, during and post-heating. Au nanoparticles are not removed from the final product material. (B) SEM images indicating Au nanoparticles adjacent to the resulting products. Au nanoparticles are not reacting with the sample. (C) Energy-dispersive X-ray (EDX) spectrum of diamond that is ion-milled from the whole sample in the gasket. Au was avoided for TEM measurements for more accurate analysis. The EDX spectrum confirms pure C measurements from the recovered samples, without presence of trace Au. (*Ga comes from the ion milling of the sample after the laser-heated diamond anvil cell experiments; Cu is the grid used for the TEM samples).

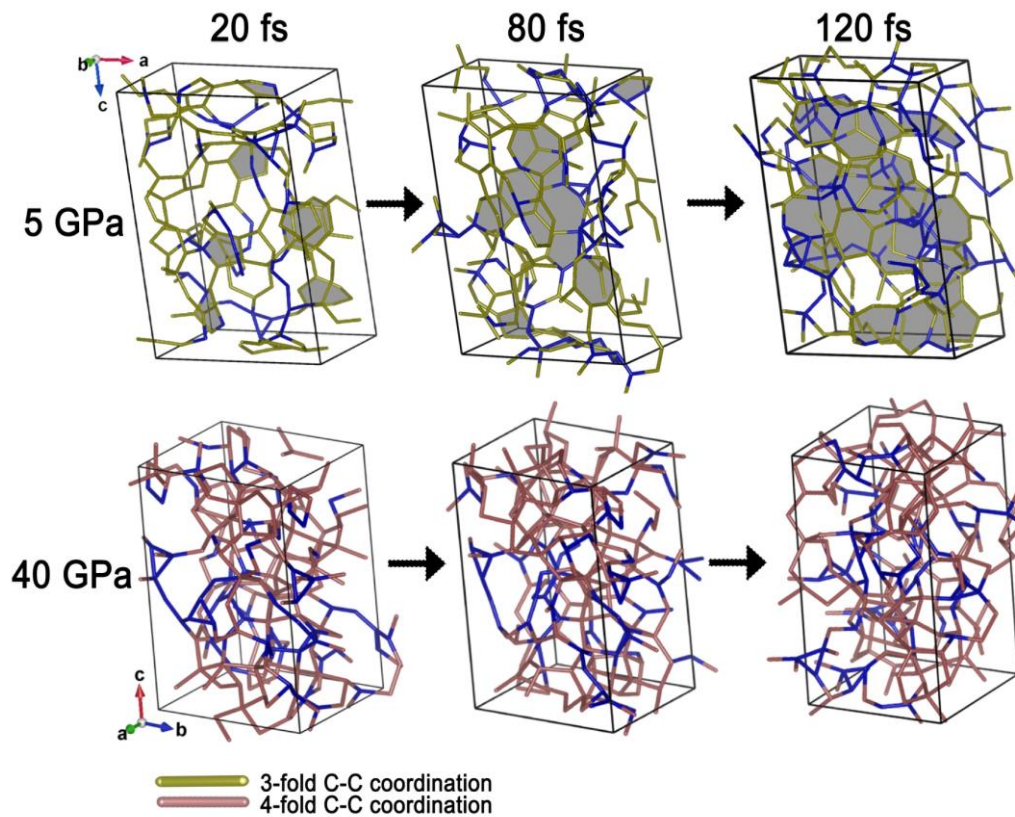
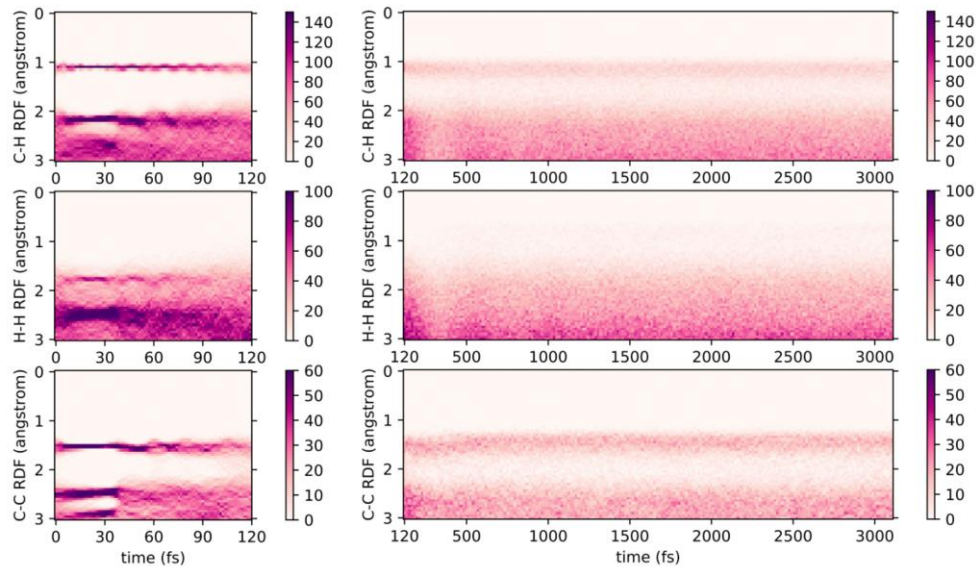


Fig. S5. Structural evolution of dehydrogenated adamantane at 5 and 40 GPa and 2000 K. Blue color represents the remaining carbon hybridization that are not sp^2 or sp^3 orbitals in 5 and 40 GPa, respectively.

A 5 GPa



B 40 GPa

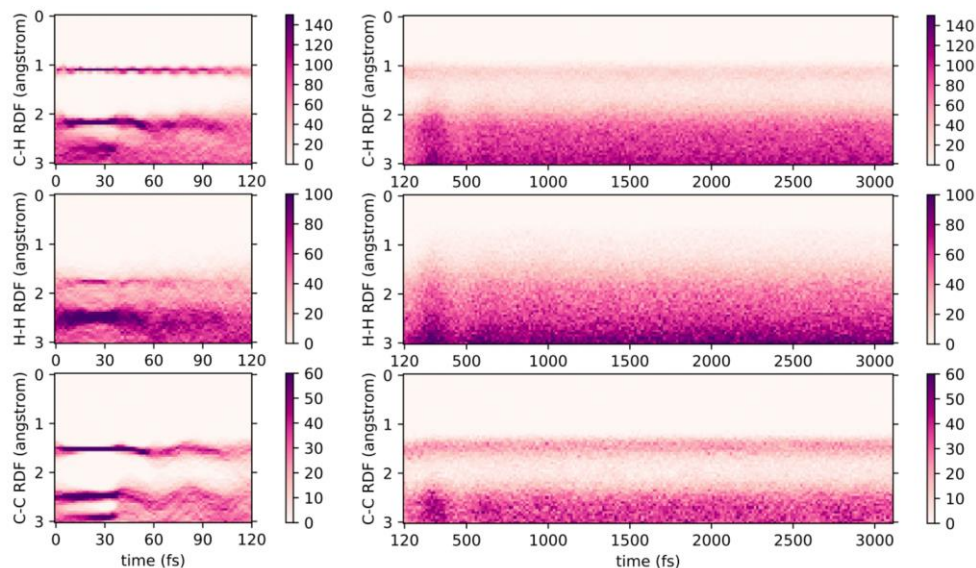


Fig. S6. False color plots indicating the calculated RDFs as a function of structural evolution time at 5 and 40 GPa. Between time 0-120 fs, the *ab initio* molecular dynamics simulation was performed with linearly-increasing temperature from 300 to 5000 K. After 120 fs, the calculation was conducted with a fixed temperature at 5000 K.

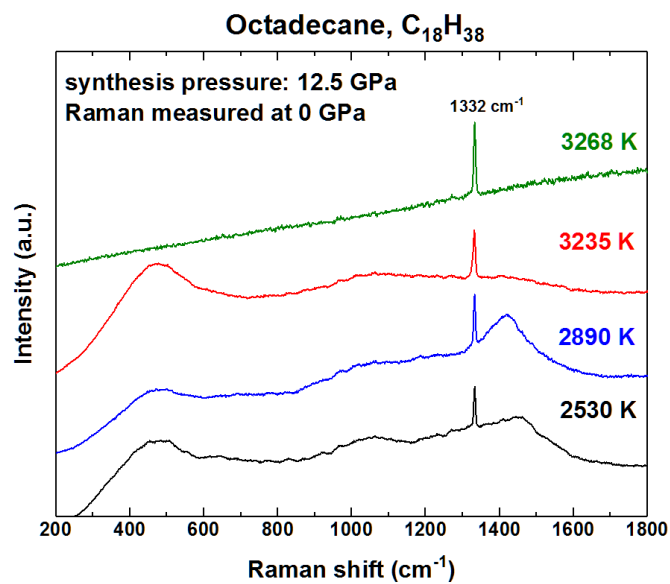


Fig. S7. Representative Raman spectra of quenched samples after laser-heating octadecane at the synthesis pressure of 12.5 GPa. Each Raman spectrum is collected from an individual laser-spot with a specific P - T value. The spectra were collected after the sample was quenched and removed from the diamond anvil cell.