Nanodiamond formation in hydrocarbons under extreme pressure–temperature conditions—Evidence from first principles

Maitrayee Ghosh[1,2], Shuai Zhang[1], and Suxing Hu[1]*

University of Rochester, [1]Laboratory for Laser Energetics and [2]Department of Chemistry

Hydrocarbons subjected to extreme conditions of pressures and temperatures widely exist in the deep interiors of giant icy planets and when used as ablators in inertial confinement fusion. Simulations using density functional theory-molecular dynamics (DFT-MD) do not show a spontaneous phase separation into diamond and hydrogen from a homogeneous C–H mixture at high pressures and temperatures below the diamond melting curve. However, DFT-MD simulations for a mechanical mixture of diamond and hydrogen showed their co-existence at 4000 K and 140 GPa. We found that the surface effect is essential to the formation of nanodiamonds in hydrocarbons at extreme conditions. Adsorption of hydrogen atoms on diamond surface decreases the free energy of the diamond–hydrogen mechanical mixture and stabilizes nanodiamonds. Our present results for C:H (1:1) are congruent to the findings of the double-shock experiments on polystyrene [Kraus *et al*., Nature Astronomy1:606–611 (2017)] which also indicate diamond formation at the same P–T conditions.

*****This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856, the University of Rochester, and the New York State Energy Research and Development Authority.