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Diamond Formation from Hydrocarbons in Planetary Conditions: An ab initio Study MAITRAYEE GHOSH, Laboratory for Laser Energetics and Department of Chemistry, University of Rochester, S. X. HU, Laboratory for Laser Energetics, University of Rochester — Shock-wave experiments have indicated the formation of diamond from polystyrene under planetary interior thermodynamic conditions (P ~150 GPa, T ~5000 K), yet a theoretical understanding still remains far-fetched.[1] [2]In this work, we have applied a reverse strategy based on quantum molecular-dynamics (QMD) simulations to demonstrate that a diamond-hydrogen separated phase is indeed more energetically favorable than a randomly mixed $(C_8H_8)_n$ system at the said thermodynamic conditions. Our QMD simulations show that hydrogen atoms should remain outside the diamond and not within its interstitial spaces. Hydrogen atoms, if present inside, will escape out and destroy the diamond structure. Depression of the melting curve of diamond also occurs because of increased C–H chemical bonding. We are now constructing a P–T phase diagram (up to T ~9000 K and P ~500 GPa) of $(C_8H_8)_n$. This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856.

[1]D. Kraus *et al.*, Nat. Astron. **1**, 606 (2017).

[2]D. Kraus *et al.*, Phys. Plasmas **25**, 056313 (2018).

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