Atomistic structure and anomalous heat capacity of low-density liquid carbon: molecular dynamics study with machine learning potential

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Liquid carbon remains the source of several unsolved questions related to its structure and region of thermodynamic stability. Experiments demonstrate a drastic decrease in the density for liquid carbon along the graphite melting line in the pressure range $P =$ 1–3 GPa and the nature of this phenomenon is unclear. A recent experimental study [1] revealed another peculiar yet unexplained feature of the liquid carbon—its excessive heat capacity. Using classical molecular dynamics with machine learning potential GAP-20 [2], we study the structural properties of liquid carbon and demonstrate that at P<1-2 GPa it resembles a net of *sp*-hybridized chains, rather than a typical covalent liquid, with nanoscale porosity of this phase being responsible for the density decrease. We also show that excessive heat capacity could be a direct manifestation of a smooth transition from a high-density sp^2-hybridized phase into a low-density *sp*-hybridized [3].

[1] Kondratyev A and Rakhel A 2019 *Physical review letters* **122** 175702
[2] Rowe P, Deringer V L, Gasparotto P, Csányi G and Michaelides A 2020 *The Journal of Chemical Physics* **153** 034702
[3] Orekhov N and Logunov M 2022 (in press) *Carbon*