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Role of sp^3 Defect in Ordered Nanoporous Carbon ENSHI XU, ANGELA LUEKING, VINCENT CRESPI, PAUL LAMMERT, Pennsylvania State Univ, KATHLEEN MALESKI, Washington College — Schwarzite is considered an ideal model for nanoporous carbon and is energetically more stable than fullerene. However, carbon don't form well-ordered Schwarzite-type nanoporous material possibly due to kinetic arrests under pyrolytic conditions. We computationally discovered a new thermodynamically stable local defect in carbon sp^2 networks: an sp^3 carbon defect, which inspires new solutions to the problem. The defect is most stable in nanoporous carbon (i.e., networks with negative curvatures, known as Schwarzites) and its topological merit, carrying negative curvature, results in the design of new model structures of nanoporous materials (periodic, negatively-curved networks), and provides a handle of the negative curvature carrier in nanoporous carbon, and we propose a kinetics-dominated synthetic route to novel nanoporous carbon with long range order by controlling the sp^3 defect through sp^3 carbon atom injection or Si atom substitution, with the aid of first principle molecular dynamics simulation. Calculations also suggest the defect can be observed by Raman.

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