Formation and Stability of Cellular Carbon Foam Structures: An *Ab Initio* Study*

David Tománek[1,*] and Zhen Zhu[1]

1 Physics and Astronomy Department, Michigan State University, USA

Inspired by the observation of an unusual structure on top of amorphous carbon covered by a thin metal layer [1], we studied the formation and structural as well as thermal stability of cellular foamlike carbon nanostructures using *ab initio* density functional calculations. The postulated structures with a mixed sp^2/sp^3 bonding character may be viewed as bundles of carbon nanotubes fused to a rigid contiguous 3D honeycomb lattice that can be compressed rather easily. The foam may accommodate the same type of defects as graphene, and its surface may be stabilized by terminating caps. We postulate that the foam may form under nonequilibrium conditions near grain boundaries of a carbon-saturated metal surface [2].

* Supported by the National Science Foundation Cooperative Agreement No. EEC-0832785, titled "NSEC: Center for High-rate Nanomanufacturing". Email of the corresponding author: *tomanek@pa.msu.edu*

[1] Julio A. Rodríguez-Manzo, Arkady V. Krasheninnikov, Zhen Zhu, David Tománek, and Florian Banhart (unpublished).
[2] Zhen Zhu and David Tománek, *Formation and Stability of Cellular Carbon Foam Structures: An Ab Initio Study*, Phys. Rev. Lett. 109 (2012) 135501.