Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Atoms dictating shape: The discrete geometry of conformal two-dimensional materials MEHRSHAD MEHBOUDI, KAINEN UTT, Univ of Arkansas-Fayetteville, HUMBERTO TERRONES, Rensselaer Polytechnic Institute, ALEJANDRO PACHECO, Universidad del Norte, EDMUND HARRISS, SALVADOR BARRAZA-LOPEZ, Univ of Arkansas-Fayetteville — The electronic, optical, thermal, mechanical and chemical behavior of two-dimensional (2D) materials depends on their shape (geometry). 2D materials are *nets* [1], with covalent bonds representing edges, and where atoms are vertices. Here we use a mathematical language to tell the shape of meshes and discuss the geometry of 2D materials of varied lattice structures, such as: hexagonal boron nitride, black phosphorus monolayers, low-buckled silicene, germanene, blue phosphorous, newly predicted III-V buckled 2D compounds such as AlP, conformal "thicker" layered materials such as 2D tin, "single-layer" transition metal dichalcogenides (MX_2's), and a single-quintuple-layer of the topological insulator Bi_2Se_3. We characterize the geometry of each atom position without recourse to a continuum parametric model. The new framework generalizes the discrete geometry we introduced recently for graphene [2,3]. References: 1. Discrete Differential Geometry, edited by A. I. Bobenko, P. Schroder, J. M. Sullivan, and G. M. Ziegler, Oberwolfach Seminars Vol. 38 (Springer, Berlin, 2008), 1st ed. 2. Pacheco Sanjuan, A. A., Mehboudi, M., Harriss, E. O., Terrones, H., & Barraza-Lopez, S. ACS Nano 8, 1136-1146 (2014). 3. Sanjuan, A. A. P., Wang, Z., Imani, H. P., Vanević, M., & Barraza-Lopez, S. PRB 89, 121403(R) (2014).

Mehrshad Mehboudi
Univ of Arkansas-Fayetteville

Date submitted: 14 Nov 2014 Electronic form version 1.4