Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Magicity of Transition Metal Nanoclusters Based on Generalized Wulff Construction SHUNFANG LI, XINGJU ZHAO, School of Physics and Engineering, Zhengzhou University, Zhengzhou, Henan 450001, China, X.S. XU, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China, Y.F. GAO, Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN, ZHENYU ZHANG, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China — Nanoclusters with extra stability at certain cluster sizes are known as magic clusters which may exhibit exotic properties. Two dominant mechanisms have been invoked to define the magicity: electronic shell closure for simple and noble metal clusters, and atomic shell closure for rare-gas and other clusters. The latter mechanism is inherently rooted in the classic Wulff construction, which stipulates that the preferred structure of a cluster should minimize its total surface energy, resulting in close-shelled icosahedronal transition metal (TM) clusters with magic sizes of 13, 55, and 147. Here we use TM clusters around 55 as examples to demonstrate that the Wulff construction must be generalized to also include the contribution of edge atoms. Specifically, a majority of the TM_{55} clusters are found to be fcc or hcp crystal fragments with much fewer edge atoms than the icosahedrons, and the magic number is shifted to its nearby even numbers. The generalized Wullf construction established here should be instrumental in fabricating nanoclusers with desirable functionalities.

Shunfang Li
Zhengzhou Universtiy, Zhengzhou, China

Date submitted: 12 Nov 2012 Electronic form version 1.4