Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Predicting Novel Bulk Metallic Glasses via High- Throughput Calculations[1] E. PERIM, Duke University, D. LEE, Harvard University, Y. LIU, Yale University, C. TOHER, Duke University, P. GONG, Y. LI, Yale University, W. N. SIMMONS, O. LEVY, Duke University, J. VLASSAK, Harvard University, J. SCHROERS, Yale University, S. CURTAROLO, Duke University — Bulk metallic glasses (BMGs) are materials which may combine key properties from crystalline metals, such as high hardness, with others typically presented by plastics, such as easy processability[1]. However, the cost of the known BMGs poses a significant obstacle for the development of applications, which has lead to a long search for novel, economically viable, BMGs[2,3]. The emergence of high-throughput DFT calculations, such as the library provided by the AFLOWLIB consortium[4], has provided new tools for materials discovery. We have used this data to develop a new glass forming descriptor combining structural factors with thermodynamics in order to quickly screen through a large number of alloy systems in the AFLOWLIB database, identifying the most promising systems and the optimal compositions for glass formation. [1] M. F. Ashby, A. L. Greer. Scripta Mater. 54, 321 (2006). [2] A. Inoue Bulk Amorphous Alloys: Preparation and Fundamental Characteristics, Vol. 4. (Trans Tech Publications, Zurich, 1998). [3] T. Egami, Y. Waseda. J. Non-Cryst. Solids 64, 113 (1984). [4] S. Curtarolo et al. Comp. Mater. Sci. 58, 218 (2012).

[1]National Science Foundation (DMR-1436151, DMR-1435820, DMR-1436268)

Eric Perim Martins
Duke University

Date submitted: 03 Nov 2015 Electronic form version 1.4