## Abstract Submitted for the MAR16 Meeting of The American Physical Society

A high-throughput search for new ternary superalloys<sup>1</sup> CHANDRAMOULI NYSHADHAM, JACOB HANSEN, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA., COREY OSES, Center for Materials Genomics, Duke University, Durham, North Carolina 27708, USA., STEFANO CURTAROLO, Center for Materials Genomics, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University, Durham, North Ca, GUS HART, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA. — In 2006 an unexpected new superalloy,  $Co_3[Al,W]$ , was discovered[1]. This new alloy is cobalt-based, in contrast to conventional superalloys, which are nickel-based. Inspired by this new discovery, we performed first-principles calculations, searching through 2224 ternary metallic systems of the form  $A_3[B_{0.5}C_{0.5}]$ , where A = Ni/Co/Fe and [B, C] = all binary combinations of 40 different elements chosen from the periodic table. We found 175 new systems that are better than the Co<sub>3</sub>[Al, W] superalloy. 75 of these systems are brand new—they have never been reported in experimental literature. These 75 new potential superalloys are good candidates for further experiments. Our calculations are consistent with current experimental literature where data exists.

[1] Sato et, al., "Cobalt-base high temperature alloys. Science 2006; 312 (5770):90-1."

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