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A high-throughput search for new ternary superalloys¹ CHANDRAMOULI NYSHADHAM, JACOB HANSEN, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA., COREY OSES, Duke University, Durham, North Carolina., STEFANO CURTÁROLO, 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, Co₃[Al, W], was discovered[1]. The new alloy is a cobalt-based alloy, in contrast to conventional superalloys which are nickel-based. Inspired by this new discovery, we performed first-principles calculations to explore many more potential superalloys. Searching through 2224 ternary metallic systems of the form A₃[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 Co₃[Al, W] superalloy. 75 of these systems are brand new— They have never been reported in experimental literature. Our results show that, in general, 1) Ni-based superallovs are more thermodynamically stable than Co- or Fe-based ones; 2) Co-based alloys have better bulk modulus than Ni- or Fe-based ones. Our results are also in agreement with the current experimental literature where they overlap. The 75 new candidates found in this work contain potential superalloys and are good candidates for performing further experiments. [1] Sato et, al., "Cobalt-base high temperature alloys. Science 2006; 312 (5770):90-1."

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