Computationally directed discovery of bismuth based binary intermetallic materials

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Bismuth based intermetallic materials display an astounding array of exotic properties, from non-trivial topology in Na3Bi, to permanent magnetism in MnBi and superconductivity in NiBi and NiBi3. Underpinning much of this behavior is the ability of bismuth, as the heaviest nonradioactive element on the Periodic Table, to provide a source of large spin-orbit coupling when in contact with a spin bearing metal. However, due to the paucity of examples of bismuth binary intermetallic compounds, the metal-metal interactions that mediate coupling are not well understood. To gain insight into the origin of these exotic electronic and magnetic phenomena, it is necessary to discover new materials and correlate their electronic and magnetic properties with their structure. While the thermodynamic binary phases are well explored, extending our focus to mapping the phase space of metastable materials provides new opportunities to reveal compounds that challenge our understanding of emergent phenomena. To systematically explore the synthesis of metastable materials, we employed in situ diffraction techniques at high applied-pressures that serve as a tunable parameter for assessing new regions of phase space. Pressure alters the thermodynamic landscape without providing additional energy to facilitate phase changes and therefore, and may be manipulated to generate and then trap otherwise inaccessible materials. However, because the high-pressure phase space of even binary mixtures of metals is vast, we set out to direct our synthetic efforts with computational techniques. By employing high-throughput ab-initio random structure searching at different pressures, we identified promising candidate structures and the pressures at which they become stable. This directed our high-pressure in situ X-ray diffraction based experiments, resulting in the discovery of new molybdenum-bismuth intermetallic phases that form in the CuAl2 structure type. This material, MoBi2, not only represents the first known binary phases for mixtures of Mo-Bi. It also indicates the stability of this structure type for high-pressure bismuth containing intermetallic materials, providing a unique opportunity to compare how transition metal-bismuth bonds influence the electronic properties of these materials.