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**High-pressure intermetallic compounds and their properties in ambient-immiscible systems** MAXIMILIAN AMSLER, SHAHAB NAGHAVI, CHRIS WOLVERTON, Northwestern University — High-pressure synthesis has recently proven to be a promising approach for the discovery of novel compounds with exciting properties that do not exist at ambient conditions. In the majority of high-pressure studies the precursors placed in a diamond anvil cell already contain constituent elements that are known to form compounds at some condition since this is the most promising approach to avoid elemental decomposition. This common practice however limits the combinations of starting elements considered, and hence a vast chemical space remains completely unexplored at high pressure. In contrast, studying alloy systems at high pressures with severe immiscibility at ambient conditions (i.e. not forming compounds or exhibiting mutual solubility over any composition-temperature-range) is a difficult endeavor. These “ambient-immiscible” systems pose a significant materials discovery challenge since no information is available if and when inter atomic bonds will form, and what crystal structures potential compounds might have once the constituent elements are exposed to pressure. We will present the discovery of high-pressure intermetallics in bismuth-containing, ambient-immiscible binary systems and their properties using structural search and ab initio calculations.

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