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High-throughput exploration of alloying as design strategy for thermoelectrics[1] SANDIP BHATTACHARYA, GEORG MADSEN, ICAMS, Ruhr University Bochum, Germany, ICAMS COLLABORATION — The essential prerequisite of a good thermoelectric material is that it exhibits favorable thermoelectric performance. However to play a key role in solving important energy challenges, it must have innocuous constituents and be cost-effective. We will discuss a new materials design strategy based on Vegard's law to optimize the thermoelectric figure of merit, zT, in binary alloys. Using a combinatorial high-throughput formalism we have explored 300 different binary M-X(X') systems, where M is a Group 1-12 element while X (X') is Si, Ge or Sn. We have identified eight promising candidates that are constituted by non-toxic and inexpensive elements and have the potential of a high zT, in addition to being thermodynamically stable. For these selected alloy systems we shall also explore in detail the correlation between their electronic structures and thermoeletric properties, to understand the source of enhancement in their transport characteristics. Furthermore, we will discuss the descriptors used to quantify the improved thermoelectric performance and the ease of alloy formation in the candidates.

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