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Partial order-disorder transitions in thermoelectric clathrates: toward non-linear modelling of materials properties

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Intermetallic clathrate alloys are promising materials for thermoelectric applications. Their cage-like unit cell allows for tailoring the electronic properties through doping. Yet, a realistic theoretical description is hard to achieve due to the complex interplay between temperature, (dis)order and electronic properties. In this work, we show a novel approach to compute the temperature-dependent band structure of alloys and apply it to the clathrate Ba8AlxSi46-x. By doing so, we i) anticipate favorable concentration and temperature ranges for thermoelectric applications, and ii) highlight the need for improved non-linear modelling of complex materials, advancing ideas based on cluster expansion.

Poster title

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