

Abstract Submitted  
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**Systematic Phase Diagram of LiSi and LiAl compounds from Minima Hopping Method**<sup>1</sup> ALDO ROMERO, Physics Department, West Virginia University, MIGUEL MARQUES, SILVANA BOTTI, RAFAEL SARMIENTO-PÉREZ, ILM, Université Lyon, IRAIS VALENCIA-JAIME, CINVESTAV, Queretaro, MAX AMSLER, STEFAN GOEDECKER, Physics Department, Basel University — We performed an extensive theoretical exploration of the structural phase diagram of LiSi and LiAl alloys through global structural prediction. These compounds have very interesting properties. For example, LiSi alloys have been considered for high energy density anodes for future rechargeable battery technology, while LiAl alloys are expected to have applications in the field of structural components due to its light weight and malleability. The global structural prediction was performed with the minima hopping method. In this method the low energy structures are obtained by solving a set of dynamical equations of motion that allows efficient visits to local minima on the Born Oppenheimer surface. We found very good agreement between our simulations and previously reported stoichiometries. Moreover, we were able to identify several novel thermodynamically stable compositions that have not been previously synthesized. The ground-state structures were further characterized both structurally and electronically. Our calculations show that global structural prediction is a very powerful tool to predict new thermodynamically stable materials, and that it consistently outperforms other methods commonly used.

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Aldo Romero  
Physics Department, West Virginia University

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