Abstract Submitted
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Lithium-Silicon crystal structure prediction by minima hopping method I. VALENCIA-JAIME, West Virginia University, R. SARMIENTO-PÉREZ, S. BOTTI, M.A.L. MARQUES, Institut Lumiere Matiere, A.H. ROMERO, West Virginia University — A throughput structural prediction of the lowest energy configurations for Li-Si alloys is presented by means of the Minima Hopping Method [1]. A convex hull is reported and compared with previous calculations and experimental structures. Unit cells with at most sixteen atoms were considered. In particular, we have found eight crystal structures lying on the convex hull. We reproduce the Li5Si2 (R-3m), as foreseen in previous theoretical calculations [2]. Additionally, we predict the thermal and elastic stability of Li3Si2 (C12/m1), Li2Si (C12/m1), Li9Si4 (C12/m1), Li3Si (P12/m1), Li7Si2 (P-3m1), Li4Si (I4/m), Li5Si (P-3m1) and Li6Si (R-3m), structures that have not been previously reported. The potential-composition curve based on those structures is also calculated and compared with previous calculations and experimental measurements.

[1] S. Goedecker, The Journal of chemical physics 120, 9911 (2004).
[2] W. W. Tipton, et. al, Physical Review B 87, 184114 (2013)

Mallory Molina
Pennsylvania State Univ

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