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First-Principles Study of Sodium Intercalation in Crystalline $Na_x Si_{24}$ ($0 \leq x \leq 4$) as Anode Material for Na-ion Batteries

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The search for Si-based anodes capable of undergoing low volume changes during electrochemical operation in rechargeable batteries is ample and active. Here we focus on crystalline Si_{24}, a recently discovered open-cage allotrope of silicon, to thoroughly investigate its electrochemical performance using density functional theory calculations. In particular, we examine the phase stability of Na_xSi_{24} along the whole composition range ($0 \leq x \leq 4$), volume and voltage changes during the (de)sodiation process, and sodium ion mobility. We show that Na_xSi_{24} forms a solid solution with minimal volume changes. Yet sodium diffusion is predicted to be insufficiently fast for facile kinetics of Na-ion intake. Considering these advantages and limitations, we discuss the potential usefulness of Si_{24} as anode material for Na-ion batteries.

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