
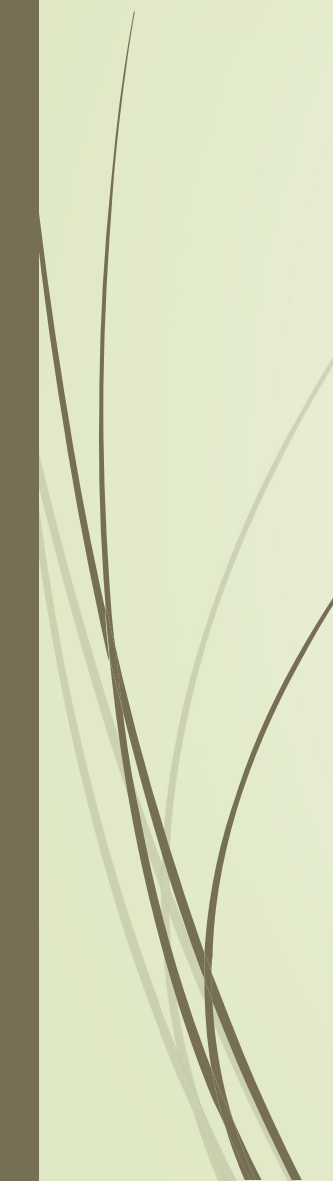


Mechanical, acoustical, and optical properties of several Li-Si alloys: a first-principles study

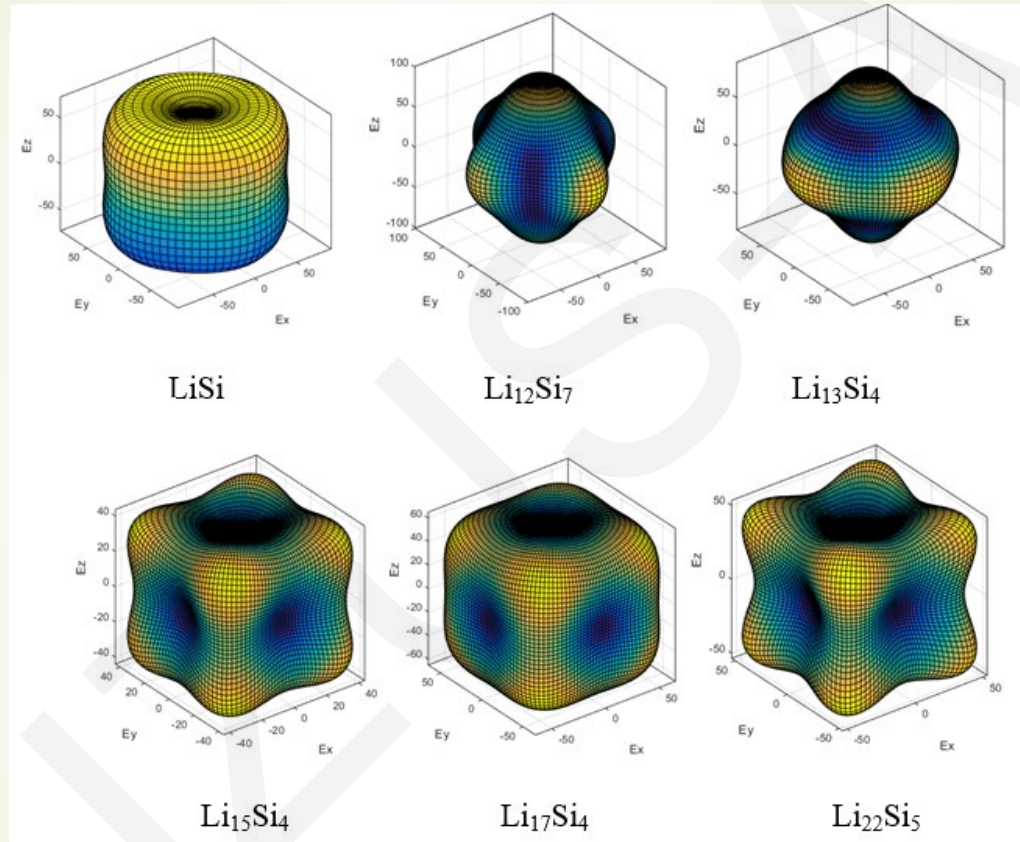
Key words: Mechanical properties; Thermal conductivity; Lithium-ion batteries; Elastic anisotropy; First-principles calculations

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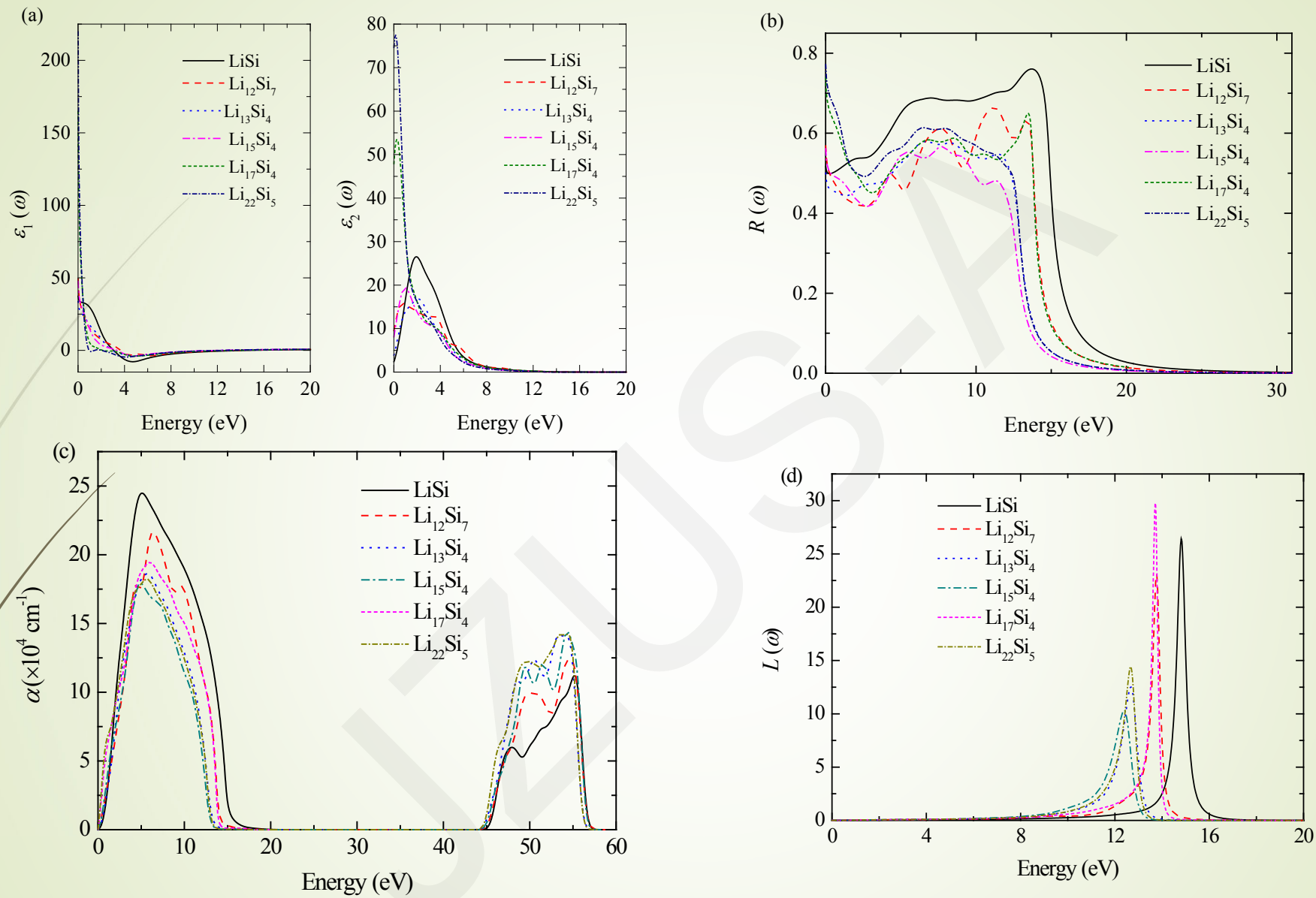
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- ▶ Li-Si alloys are potential candidates for the next-generation of high energy-density anode materials for rechargeable lithium-ion batteries (libs) because of silicon can host lithium.
 - ▶ Research has shown that the Li-Si alloy suffers capacity fade and does not form a stable solid electrolyte interphase layer, so it is of importance to explore mechanical, acoustical and optical properties of Li-Si phases in order improve battery performance.

RESULTS



- Figure 1 The three-dimensional dependence of the young's modulus of the studied li-si alloys. E_x , e_y , and e_z are the three components of young's modulus along the x, y, and z .



➤ Figure 2 The optical properties of the studied li-si alloys. (a) dielectric functions; (b) the reflectivity; (c) the absorption coefficient; (d) electron energy loss spectra.

CONCLUSIONS

- These Li-Si alloys are mechanically stable and susceptible to shape deformation.
- All the studied Li-Si alloys have a significant anisotropic Young's modulus and exhibit butterfly-shaped curves on some planes.
- Debye temperature increases in the sequence $\text{Li}_{15}\text{Si}_4 < \text{LiSi} < \text{Li}_{22}\text{Si}_5 < \text{Li}_{12}\text{Si}_7 < \text{Li}_{13}\text{Si}_4 < \text{Li}_{17}\text{Si}_4$.
- The longitudinal wave along the [111] direction is fastest for the cubic system, while it is the fastest along the [001] direction for the orthorhombic system and along the [010] direction for the tetragonal system.
- All the studied Li-Si alloys have relatively low thermal conductivities and are promising dielectric materials.