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Density Functional Tight-Binding (DFTB) Study of Si as an Anode Material

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Abstract content
   (Max 300 words)

Silicon is an attractive candidate amongst anode materials for rechargeable Li-ion batteries due to its highest theoretical capacity of 4200 mAhg⁻¹ in Li-Si alloys corresponding to a fully lithiated state Li₂₂Si₅. However, coupled with the attractiveness are cyclability issues, an irreversible capacity loss, and a deleterious volume expansion leading to capacity fade. Density functional tight-binding (DFTB) is demonstrated to have the plausibility as an efficient study approach for complex Si systems. We establish the reliability of the parameterization scheme by showing that the simulation results of structural properties for Si, Li, Li-Si compare well with available experimental and first principle results to within less than 5% difference. The ability of the tight-binding method to study Si systems is illustrated by using molecular dynamics to calculate thermal and electronic properties of Si with simulation unit cells of up to 512 atoms. Molecular dynamics results confirm DFTB as a feasible computational approach for Si systems.

Apply to be
 consider for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD)?

Hons

Main supervisor (name and email)
and his / her institution

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Would you like to <br> submit a short paper <br> for the Conference
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No

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