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Self-Consistent Charge Density-Functional Tight-Binding Parameterization for the Mg–Si system

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Lithium-ion batteries have been widely used as a solution for portable energy storage over the years, however, the rising demand for high-energy-density batteries calls for the design of new high-performing electrode materials. Magnesium-based batteries emerged among alternatives to lithium-ion batteries, however, further studies are still required to help accelerate developments toward their commercialisation. In this work, we present the self-consistent charge density-functional tight-binding (SCC-DFTB) parameterization of the Mg-Si system. The developed parameters are validated against available experimental data and calculated DFT results using Mg, Si and Mg-Si systems. The structural properties obtained by applying the parameter set show good agreement with the experimental values, and by modelling the electronic properties of the Mg₂Si supercell the set is shown to handle large systems. The Mg-Si SCC-DFTB parameters from this work paves the way for further investigations, as they will make it possible to study and predict the behaviour of Mg-Si-based electrode materials through computer simulations.

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No

Level for award;(Hons, MSc, PhD, N/A)?

N/A

Primary authors: Mr MAPHANGA, Simon; Dr PHOSHOKO, Katlego (University of Limpopo); NGOEPE, Phuti (University of Limpopo)

Presenter: Dr PHOSHOKO, Katlego (University of Limpopo)

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