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Structural, electronic and optical properties of rare-earth copper chalcogenides LaCuX₂ (X = S, Se): A first principles study

Thursday, 11 July 2019 15:00 (2 hours)

Structural, electronic and optical properties of rare-earth copper chalcogenides LaCuX₂ (X = S, Se) were investigated with density fuctional theory (DFT). The calculated structural properties agree resonably well with previous results and experimental data. Elastic constants satisfy the stability conditions for monoclinic structures, wich confirms mechanical stability for the compounds. Modified Becker Johnson (MBJ) potential band structure and density of state calculation reveals that LaCuX₂ (X = S, Se) are indirect band gap semiconductors with DFT energy gaps between 1.30 to 1.50 eV. The fundemental gaps were determined at G₀W₀ level of approximation, while optical parameters such as dieclectric functions, refractive indices, energy loss functions and absorption coefficients were examined by solving the Bether Selpater equation. From the results obtained, LaCuX₂ are stable compounds and posses energy gaps suitable for photovoltaic applications.

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

yes

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

PhD

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