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A Theoretical Investigation of the Structural, Electronic and Phase transition of Molybdenum Selenide compounds

Tuesday 09 Jul 2013 at 17:40 (01h00')

Abstract :

Molybdenum selenide structures may be potential may be potential materials for constructing solar cells. In this study, we numerically investigate the structural, electronic structure and pressure phase transition properties of some molybdenum selenide structures using density functional theory (DFT). Three DFT approximations are used to determine trends and properties. Pressure phase transitions up to 10 Gpa and elastic properties are examined to identify structurally stable systems. The electronic structure of the most stable systems are explored to determine the best potential candidates for solar energy harvesting.

Award :

Yes

Level :

PhD

Supervisor :

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Paper :

No

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