Ab-initio investigations of LuLiF4 compound under pressure

Petrova A., Minisini B., Nedopekin O., Tayurskii D. Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

We have performed ab-initio calculations for the structural and mechanical properties of sheelite compound LuLiF4 under pressure. A good agreement with experimental results has been obtained.

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