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Mechanical properties of Y2SiO5-Lu2SiO5 solid solutions from ab initio calculations

Yttrium orthosilicate (Y_2Si2O_5 or YSO) is one of the scintillator materials that is successfully used in Compact Muon Solenoid (CMS) detectors in the Large Hadron Collider. This material can be chemically modified by substituting yttrium Y^{3+} metal ion(s) with lutetium Lu^{3+} ions, resulting in a range of compositions represented by the formula $Lu_xY_{(1-x)}SiO_5$, Lu_2SiO_5 (LSO). Additionally, cerium Ce^{3+} ions can be introduced as impurities into the crystalline lattice at varying concentrations. Oxy-orthosilicate materials exhibit the excellent radiation resistance and favourable luminescence properties.

In this work we study YSO-LSO solid solutions using group action theory for structure generation and *ab initio* approach for calculating equilibrium crystal structures and their corresponding elastic properties. The simulated solid solutions employed a 32-atom primitive cell featuring eight yttrium atoms. We explored nine compositions, varying the lutetium content from 0% to 100% in increments of 12.5%. A total of 74 symmetry-independent structures were generated and analyzed. For each composition, solutions with the lowest total energy were identified. Certain compositions displayed multiple energetically similar solutions, differing by only tens of milli-electron volts (meV) per primitive cell.

Our findings reveal that the volume of the crystallographic unit cell exhibits an almost linear decrease as the lutetium content increases. However, the composition with 37.5% Lu deviates significantly from this linear trend, warranting further in-depth analysis. The bulk modulus displays a distinct pattern, increasing from approximately 92 GPa for pure YSO to around 120 GPa for a 50% LYSO mixture, before slightly decreasing to about 115 GPa for pure LSO.

The results obtained are consistent with available structural data and contribute new insights into the mechanical properties of these materials. Such findings could be pivotal for future advancements in high-energy physics and related fields.

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Type of contribution

Poster

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