Contribution ID: **93** Type: **Student Micro-talk**

First-principle study of monazite systems

Monazite is an important mineral in the mining industry and contains non trivial amounts of rare earth elements (REEs), thorium (Th) and uranium (U). These components are exceptionally significant and find application in numerous areas of modern technology and are generally used in catalysis, metallurgy and magnetic sector. The thermal plasma treatment is a new process of high-temperature cracking that is being investigated to improve the extraction of REEs, Th and U from monazite. The stability of monazite structures was investigated using first-principle density functional theory (DFT) to understand the cracking process. The calculated lattice parameters of monazite were found to be within 5% in good agreement with the experimental values. Furthermore, it was found that all structures in monazite showed negative for C35, a condition of mechanical instability. It was also found that monazite type structures showed a ductile behaviour. The findings provide an understanding of the monazite that may be helpful in plasma cracking optimisation experimental methodologies.

HPC content

First-principle study of monazite systems were achieved by using VASP code in the Medea environment at the CHPC

The structural, thermodynamic and mechanical properties were achieved by utilising the VASP code

Application code: VASP

Problem size: 24 atoms

Core count: 48

Computational challenges: currently, calculations at CHPC fail to run, I'am getting errors

Student?

Yes

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