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Ab-initio structural and mechanical stability study of the uranium – aluminium alloys (UAl2, UAl3 and UAl4)

We use DFT calculations within GGA-PBE approximation to investigate the structural and mechanical stability of uranium-aluminium systems. Our results provided excellent heats of formation and predict UAl2 to be more stable, in agreement with experiment. Phonon dispersion spectra confirmed relative structural trend, all three compounds where mechanical stability

Primary author: Mr MOTSWARE, Teboho Cyprian (Student)

Co-authors: Dr CHAUKE, Hasani Richard (Member); Prof. NGOEPE, Phuti (Member)

Presenter: Mr MOTSWARE, Teboho Cyprian (Student)

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