Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Density-Functional and CALPHAD Studies of U-Zr Alloys
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The U-Zr alloy alloys have been recognized as a fuel for liquid-metal fast breeder reactors. First-principles methods are employed to study ground-state properties of U-Zr alloys for the most important phases observed experimentally, namely γ (bcc) and δ (C32). Effective interatomic interactions obtained from the screened GPM, incorporating KKR-ASA-CPA, have been applied in MC simulations to derive the γ-phase miscibility gap. EMTO-CPA method has been applied to study properties of the open δ-phase. Results of *ab initio* calculations are compared with experimental data and CALPHAD assessment. Then, the CALPHAD assessed U-Zr phase diagram is contrasted with the one predicted with the input from *ab initio*. This work shows that an overall validity of a combined *ab initio*–CALPHAD approach to thermodynamic properties exists, and that the knowledge and quantitative output gained from quantum mechanics on phase stability and its relation to f-bonding, can be used to explore other actinide-based systems, for which experimental data are sparse or lacking. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Date submitted: 27 Nov 2007 Electronic form version 1.4