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Density-functional study of U-Mo alloys ALEXANDER LANDA, PER SODERLIND, PATRICE E.A. TURCHI, Lawrence Livermore National Laboratory, Livermore, USA — The U-Mo and U-Zr alloys proved to be very promising fuels for advanced fast nuclear reactors. According to numerous experiments, the main advantages of U-Mo fuels over U-Zr fuels lies in a much lower constituent redistribution due to the existence a single γ-U-Mo phase with body-centered cubic structure over typical fuel operation temperatures. Density-functional theory (EMTO-CPA technique) previously used to describe phase equilibria in U-Zr alloys [A. Landa, P. Söderlind, P. E. A. Turchi, Journal of Alloys and Compounds, 478 (2009) 103] is extended to investigate the ground-state properties of U-Mo solid solutions. Calculated heats of formation of bcc U-Zr and U-Mo alloys are compared with CALPHAD assessments. We discuss how the heat of formation in both alloys correlates with the charge transfer between the alloy components, and how the specific behavior of the density of states in the vicinity of the Fermi level promotes the stabilization of the U_2Mo compound. Our calculations prove that, due to the existence of a single γ-phase over the typical fuel operation temperatures, γ-U-Mo alloys should indeed have much lower constituent redistribution than γ-U-Zr alloys for which binodal decomposition causes a high degree of constituent redistribution. This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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