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Density-functional study of the $La_2Zr_2O_7$ low-index faces YVES MANTZ, YUHUA DUAN, NETL — The (001), (011), and (111) faces of the catalytic host lanthanum zirconate ($La_2Zr_2O_7$) are studied at the level of density-functional theory (DFT), including all surfaces formed by cleaving a perfect crystal ("bulk-truncated") and a subset of defective surfaces. Surface free energies are computed, dependent on O chemical potential for (001) and (011) surfaces and O and La or Zr chemical potentials for (111) surfaces, with vibrational contributions obtained from computed atomic frequencies and/or phonon dispersions. Taking into account error in determining the conditions where a given surface is thermodynamically preferred, a relaxed defective (001) or (011) surface is shown to be preferred to any relaxed bulk-truncated (001) or (011) surface over a subset of temperatures and oxygen gas partial pressures. Thus, the existence is proven of (001) and (011) faces that cannot be relaxed bulk-truncated, e.g., are defective or reconstructed. Extending this work, the existence of a (111) face that is not relaxed bulk-truncated is addressed. The main finding, of faces that are not relaxed bulk-truncated, is discussed in the context of comparing predicted versus experimental crystallite thicknesses obtained from a data analysis.

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