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Hematite nanoribbons based on (110) and (104) surfaces and their unusual character[1] PRABATH WANAGURU, JIAO AN, QIMING ZHANG, The University of Texas at Arlington — Atomically thin hematite nanoribbons based on (110) and (104) surfaces are studied systematically by first-principles methods. Calculations have performed using the GGA+U approach and structures were fully relaxed to identify the geometric, electronic and magnetic properties. The studied hematite nanoribbons are formed by cutting the atomically-thin hematite nanosheets along their [100] and [010] directions. The (110) surface based nanoribbons show definite tunable semiconducting character while one type of the (104) based nanoribbons display surface modifications or bending nature indicating pseudo-Jahn-Teller effect. The remaining type of (104) based nanoribbons show built-in oxygen vacancy on one edge despite preserving the stoichiometry and introduces the half-metallicity into the nanoribbons at larger widths. We will present the optimized structures, their electronic properties and energetics in detail.

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