Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles studies of hematite nanoribbons[1] PRABATH WANAGURU, JIAO AN, QIMING ZHANG, The University of Texas at Arlington — A study of two types of hematite nanoribbons, based on density functional theory has been performed. Geometry and magnetic order of these nanoribbons were optimized using DFT+U method implemented in VASP suite of software. It is found that the band gaps decreases from the value of $\sim$ 2.0eV to $\sim$ 1.7eV as the widths increase from 6Å to more than 40Å. Despite the bulk hematite is indirect in band gap nature, one type of nanoribbons show direct band gap nature in several widths. Cleaving energies are positive with respect to the hematite sheet and as width increases it is decreasing. Moving from smaller width to a larger width, nanoribbons were showing more of a sheet like character. Other properties of these nanoribbons will also be discussed.

[1]This research is supported by NSF SusChEM Program (Award DMR-1306291).

Prabath Wanaguru
The University of Texas at Arlington

Date submitted: 14 Nov 2014 Electronic form version 1.4