

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Accurate projected augmented wave (PAW) datasets for rare-earth elements (RE=La-Lu)**<sup>1</sup> MEHMET TOPSAKAL, RENATA WENTZCOVITCH, Univ of Minn - Minneapolis — We provide accurate projected augmented wave (PAW) datasets for rare-earth (RE) elements with some suggested Hubbard U values allowing efficient plane-wave calculations. Solid state tests of generated datasets were performed on rare-earth nitrides. Through density of state (DOS) and equation of state (EoS) comparisons, generated datasets were shown to yield excellent results comparable to highly accurate all-electron full-potential linearized augmented plane-wave plus local orbital (FLAPW+LO) calculations. Hubbard U values for trivalent RE ions are determined according to hybrid functional calculations. We believe that these new and open-source PAW datasets will allow further studies on rare-earth materials.

<sup>1</sup>NSF/EAR 1319361

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Date submitted: 14 Nov 2014

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