Supplementary information

Evolution of valence state of Ru metal ions in correlation with structural and electronic properties of double perovskite ruthenates; A_2SmRuO_6 (where A = *Ba* & *Sr*)

Sahil Dani,[a] Rabia Pandit,[b] Hitesh Sharma,[b] A. Arya,[c] R J Choudhary,[d] Navdeep Goyal,[e] Jarnail Singh,[f] and Rakesh Kumar*[a]

[a] *Department of Physics, Indian Institute of Technology, Roopnagar, 140001, Punjab, India*

[b] *Department of Physical Sciences, IKG Punjab Technical University, Kapurthala, 144603, Punjab, India*

[c] *Glass and Advanced Materials Division, Bhabha Atomic Research Centre, Trombay, Mumbai, 400 085, India*

[d] *UGC-DAE Consortium for Scientific Research, Indore 452001, India*

[e] *Department of Physics, Panjab University, Chandigarh 160014, India*

[f] *School of engineering and technology, K R Mangalam University, Gurugram, 122103, India*

1. UV-Vis reflectance spectra

The optical band gap measurements have been carried out using Ultraviolet visible spectrophotometer model number Analytik-Jena Specord 250 PLUS in the reflectance mode.

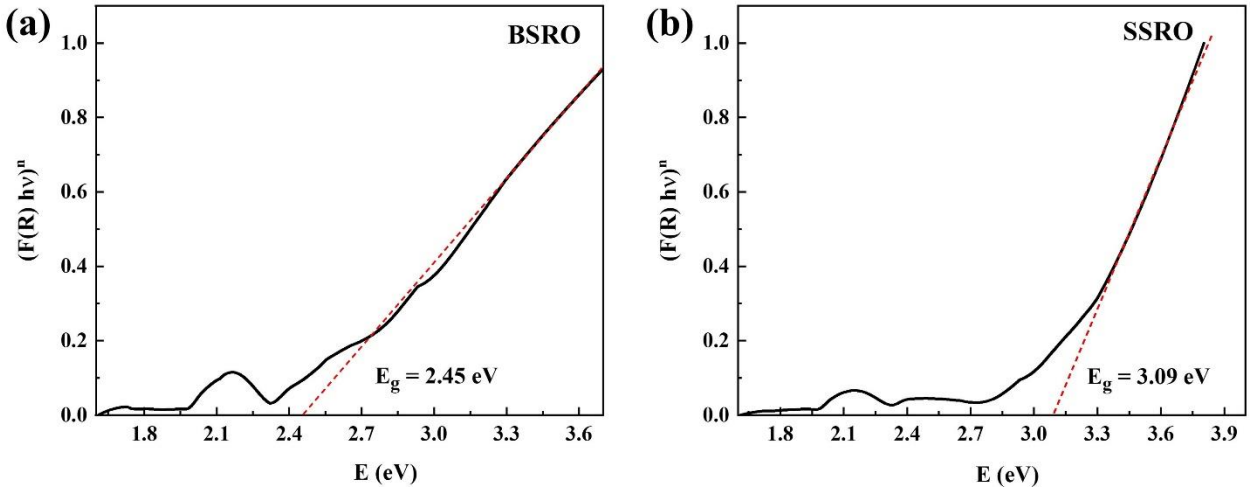

Figure S1. Kubelka-Munk function fit to the reflectance spectra to determine the optical bandgap for (a) BSRO and (b) SSRO.

2. Optimization of U parameter

For optimization of the Hubbard parameter U for the theoretical electronic structure calculations, the unit cell structure and atomic positions have been fully relaxed for a set of U values ranging from 0-10 eV for 4*d* and 4*f* electrons of Ru and Sm, respectively.

The optimum value of U has been taken, where the difference of magnetic and non-magnetic ground state with U parameter converges to zero. The optimized value of U is 7 eV for BSRO and 9 eV for SSRO (Figure S2).

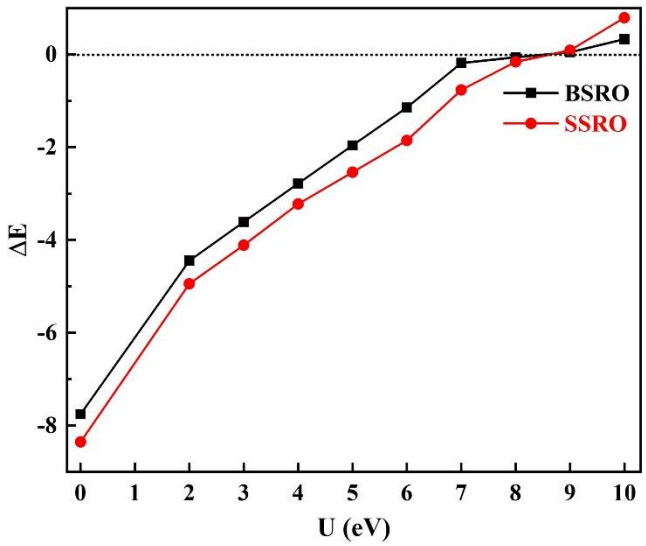

Figure S2. Difference between the ground state energy of BSRO and SSRO corresponding to their non-magnetic and magnetic state with U parameter plot as a function of U for BSRO (Black) and SSRO (Red) compounds.