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Supplementary: Electronic, Magnetic, Optical and Thermoelectric Properties of $Ca_2Cr_{1-x}Ni_xOsO_6$ Double Perovskites

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With the help of density functional theory calculations, we explored a recently synthesized double perovskite material Ca_2CrOsO_6 and found it to be ferrimagnetic insulator with a band gap of $\sim$0.6 eV. The effective magnetic moment of it is found to be $\sim$0.23 μ_B/unitcell. The proposed behavior arises from the cooperative effect of spin-orbit coupling and Coulomb correlation of Cr-3d and Os-5d electrons along with the crystal field. Within the ferrimagnetic configuration, doping of 50% by Ni to the Cr-site resulted in the half-metallic state with compensation of total moments nearly to zero, a characteristic of spintronic materials. Meanwhile, the optical study reveals that both ε_1^{xx} and ε_1^{zz} decreases first and increases rapidly with increasing photon energy up to 1.055 eV. We also found the optical anisotropy up to $\sim$14 eV, which becomes almost optically isotropic. This material has a plateau like region in the σ_{xx} and σ_{zz} part of the optical conductivity due to a strong $3d$-$5d$ interband transition between Cr and Os. In addition, we performed the thermoelectric calculations whose results predicts that the material might not be good as a thermoelectric device due to small power factor.

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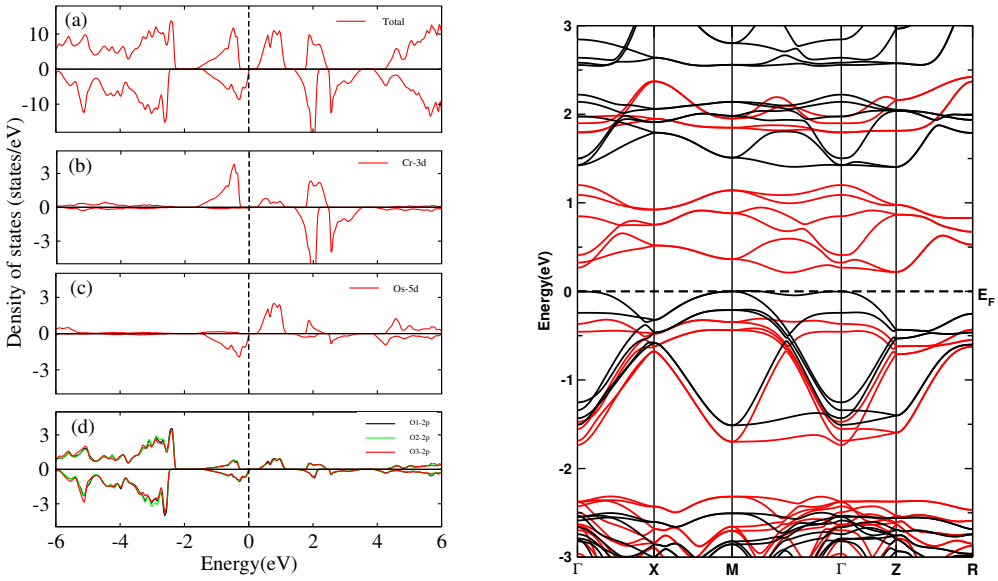

Fig. S1 (Color online) DOS (top) and band structure (bottom) of Ca_2CrOsO_6 with GGA functional. The vertical in (up) and horizontal in (down) dotted line indicates E_F=0.

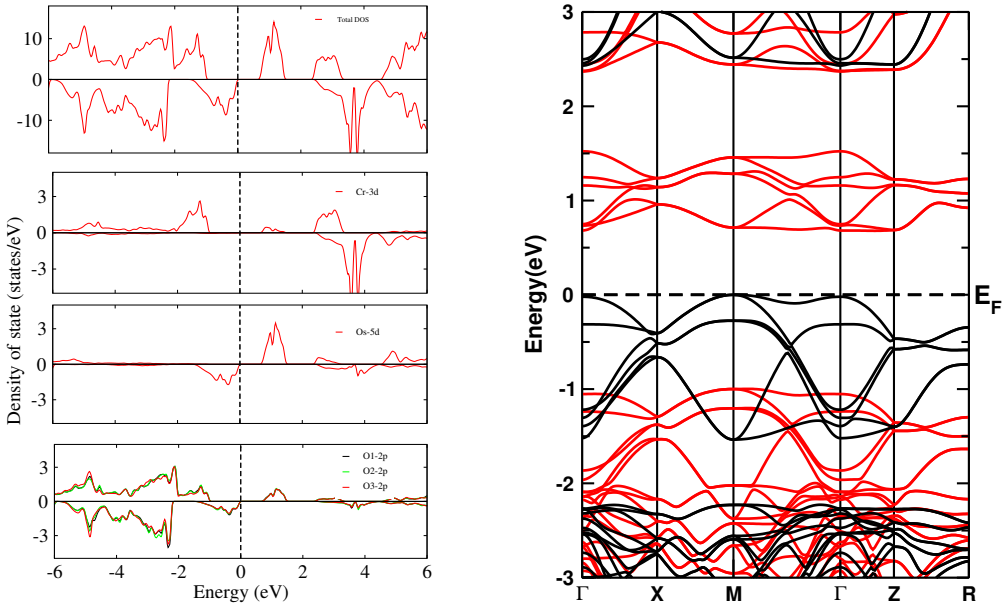

Fig. S2 (Color online) DOS (left) and band structure (right) of Ca_2CrOsO_6 with GGA+U functional. The vertical in (left) and horizontal in (right) dotted line indicates E_F=0.

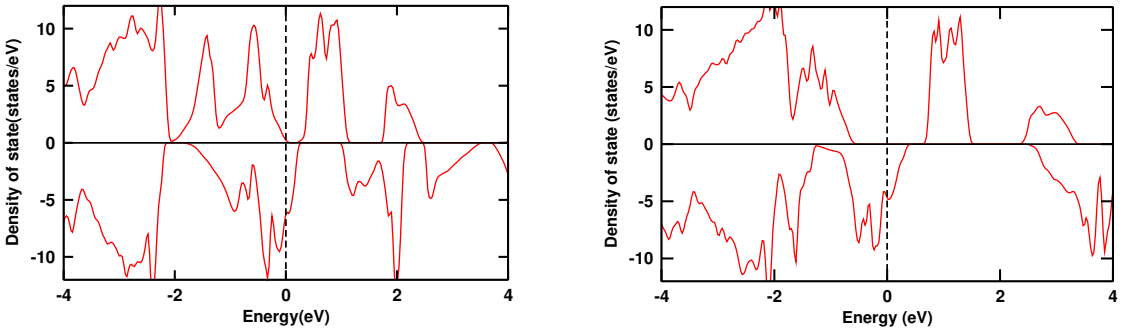

Fig. S3 (Color online) Total DOS of $Ca_2Cr_{0.5}Ni_{0.5}OsO_6$ with GGA (left) and GGA+U (right) functional. The vertical dotted line indicates E_F=0.

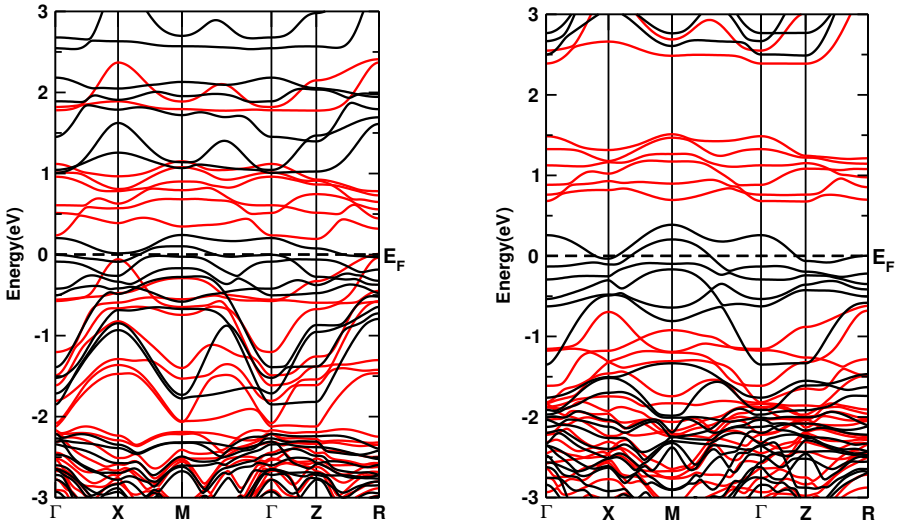

Fig. S4 (Color online) Band structure of $Ca_2Cr_{0.5}Ni_{0.5}OsO_6$ with GGA (left) and GGA+U (right) functional. The horizontal dotted line indicates E_F=0.