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Predictions for Spin Resolved Spectral Function and Optical Conductivity in Half-metallic Double Perovskites[1] JULIA JANCZAK, OINAM NGANBA MEETEI, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — We present the effects of thermal fluctuations and anti-site (AS) disorder on the spin resolved spectral function $A(k,\omega)$ and optical conductivity $\sigma(\omega)$ for half-metallic double perovskite Sr_2FeMoO_6, which holds great promise in spintronics applications. While both $T \neq 0$ and AS destroy the half metallic state, they produce distinct effects. Increasing T produces smooth broadening in the energy distribution curves of $A(k,\omega)$ while AS produces localized states at specific energies with broad momentum distribution curves for spin up. Our results can be tested directly in spin resolved ARPES experiments. We also calculate $\sigma(\omega)$ by evaluating the Kubo formula in the exact eigenstate basis. We show for $T \neq 0$ the height of the secondary peak in $\sigma(\omega)$, also seen in experiments, tracks the polarization P of conduction electrons, whereas for disordered samples at $T = 0$, the weight of the secondary peak indicates the amount of AS. From the spin resolved conductivity, we show that small ($< 10\%$) amounts of AS prevalent in real samples has little impact on the spin polarization of the DC current. The features of the optical spectrum provide a relatively simple experimental probe of the polarization and amount of disorder.

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