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Theory of Spectroscopy and Transport in Half-metallic **Perovskites¹** JULIA JANCZAK, OINAM NGANBA Double MEETEI, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — Half-metallic double perovskites hold great promise in spintronics applications, hence we are motivated to understand the spectroscopy and charge transport in these materials. We present theoretical calculations of the temperature and disorder dependence of the spin-resolved density of states of the conduction electrons, the optical conductivity $\sigma(\omega)$, and the anomalous Hall conductivity for Sr₂FeMoO₆ (SFMO), a half-metal with 100% spin-down polarized charge carriers at T = 0. We build on the recent progress [1] in modeling magnetic properties of SFMO by using an exact diagonalization plus Monte Carlo scheme. We obtain $\sigma(\omega)$ as a function of disorder as well as temperature using the Kubo formula for linear response in the exact eigenstate basis. In agreement with experiment, we find a secondary peak in $\sigma(\omega)$ at $\omega \sim 0.5 \, eV$, and attribute it to a spin-up density of states at the chemical potential induced by disorder and/or thermal fluctuations. We propose that the size of the secondary peak can be used to determine the polarization of conduction electrons at the chemical potential, facilitating experimental measurements.

[1] O. Erten et al, arXiv:1107.0983; Phys. Rev. Lett. (to appear)

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