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Electronic excitations in YTiO3[1] WILLIAM THORNTON, University of Tennessee, ANTON KOZHEVNIKOV, Oak Ridge National Laboratory, ADOLFO EGUILUZ, ROBERT HARRISON, University of Tennessee — We study the electronic excitations across the Mott gap in YTiO3 using time dependent density functional theory, implemented in a Wannier basis. The leading excitation, lying at $\sim$2eV, involves orbitally ordered states. In the optical limit, the excitation is a dipole-allowed d-d off site feature which we analyze in view of recent optical data and model calculations (PRB 76, 155125 (2007), and PRB 78, 075122 (2008)). For large wave vectors, the loss feature switches over to on-site d-d character; its strength and energy location depends sensitively on the d-d excitonic interaction. This on-site excitonic feature may be observable via inelastic scattering of x-rays.

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