Electron correlation and spin-orbit-lattice coupling in pyrochlore iridates

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The pyrochlore iridates are considered as very promising candidates for realizing exotic quantum states of matter such as Weyl semimetals and topological Mott insulators. The phase diagram is predicted to have these quantum phases over a certain range of relative correlation U/W and spin-orbit coupling λ/W [1]. We used spectroscopic ellipsometry to determine the dielectric function of $A_2Ir_2O_7$ (A = In, Lu, Y) polycrystalline samples in the wide spectral range from 10 meV to 6.5 eV at temperatures from 7 K to 300 K. Comparing the spectra with the results of relativistic LSDA+*U* band structure calculations, we quantitatively classify pyrochlore $A_2Ir_2O_7$ as spin-orbital J_{eff}=1/2 Mott insulators with the on-site Coulomb interaction U≈1.5 eV and the electronic bandwidth W = 0.3÷0.5 eV. Exciton doublets with pronounced Fano line shapes were identified in $Y_2Ir_2O_7$ and $Lu_2Ir_2O_7$ upon cooling below the magnetic ordering temperatures T_N = 150 K and 145 K, respectively. The formation of exciton complexes observed at the absorption edge is accompanied by distinct phonon anomalies in the infrared spectra. Our results indicate considerable effects of long-range Coulomb interaction and spin-orbit-lattice coupling in the 5d-pyrochlore compounds and the need for a detailed analysis of their influence on the J_{eff}=1/2 states. Newly synthesized $In_2Ir_2O_7$ does not exhibit the absorption edge and phonon anomalies below T_N = 45 K and thus serves as a reference.

References

[1] W. Witczak-Krempa, G. Chen, Y. B. Kim, L. Balents 2014 *Annu. Rev. Condens.* 5, 57.