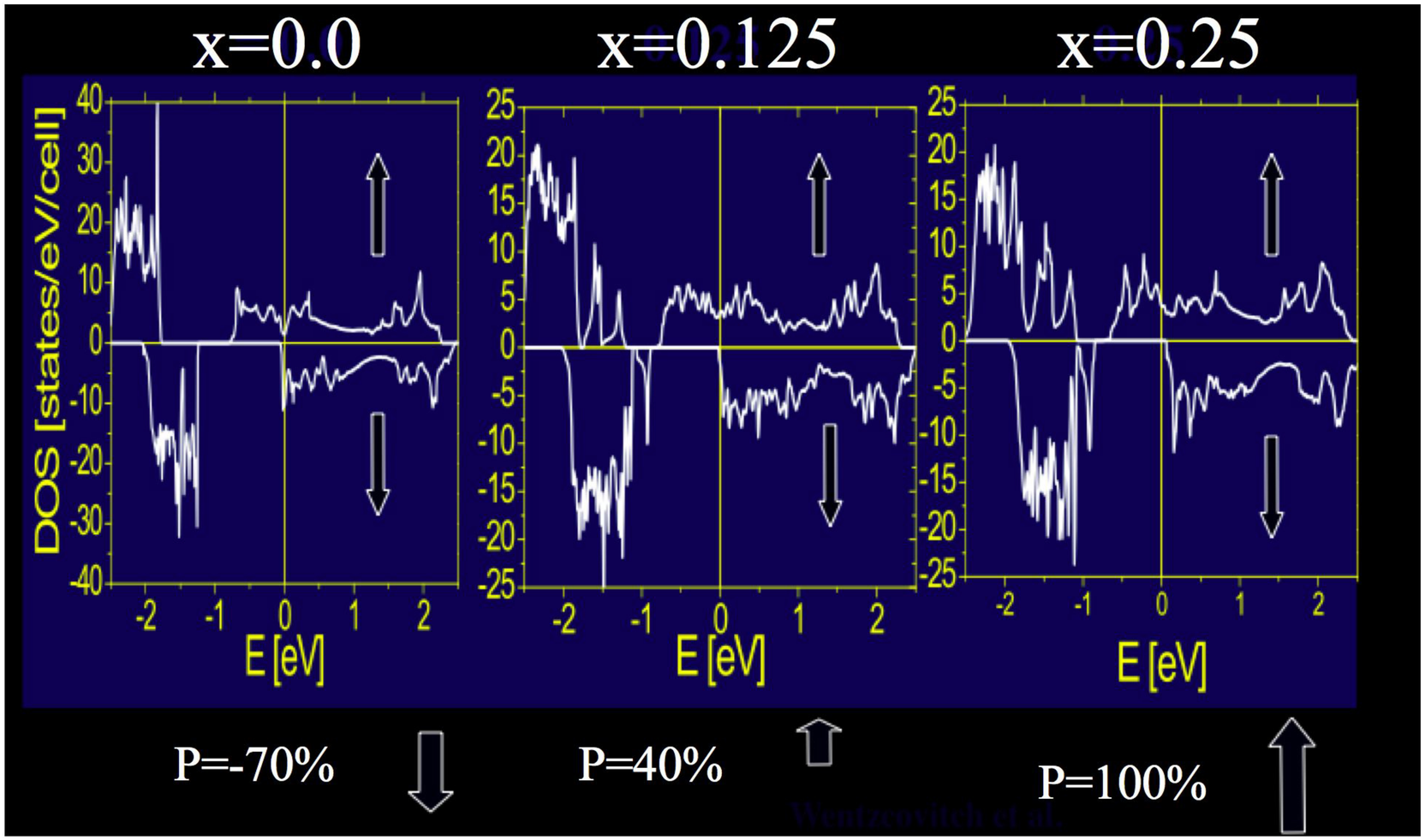
Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky, Yousef Saad and Renata Wentzcovitch (Minnesota), Steven G. Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR-0325218): Spintronic Materials



Density of states for $Co_{1-x}Fe_xS_2$. The energy zero is the Fermi-level. For x=0, the material is a ferromagnetic metal with "negative" spin polarization, i.e., the polarization at the Fermi-level is opposite to the majority spin. The change in sign of the polarization as a function of x has been observed experimentally. It was predicted before the experiment.

Spintronic materials are designed to have net spin polarization at the Fermi-level. We have been examining alloys: $Co_{1-x}Fe_xS_2$. CoS_2 is a metallic ferromagnet, FeS_2 is a diamagnetic semiconductor. By alloying the two sulfides we can change the net polarization:

$$P = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow} = 1$$

to achieve the desired properties.