Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Magnetic, magneto-optical and dielectric properties of ferromagnetic semiconductors $CdCr_2S(Se)_4$ from first-principles calculations GUANG-YU GUO[1], HAI-QING LIN, Department of Physics, Chinese University of Hong Kong, Shatin, Hong Kong — Recently, $CdCr_2S_4$ has been found to exhibit fascinating relaxor ferroelectricity and colossal magnetocapacitive effect.To understand this and other interesting properties, we have calculated the electronic structure, exchange coupling, optical dielectric constant and magneto-optical Kerr rotation of $CdCr_2S_4$ and $CdCr_2Se_4$. The calculations are based on density functional theory with generalized gradient approximation plus on-site Coulomb correlation (GGA+U). The all-electron full potential linearized augmented plane wave (FLAPW), frozen core full potential projector augmented wave (PAW), and also all-electron tight-binding linear muffin-tin orbital methods (TB-LMTO) are used. In this contribution, we will present the obtained exchange coupling parameters, magneto-optical Kerr rotation spectra and dielectric constants. In particular, we will discuss the possible origins of the obtained ferroelectricity in these materials.

[1]On sabbatical leave from Department of Physics, National Taiwan University, Taipei, Taiwan

Guang-Yu Guo
Department of Physics, Chinese University of Hong Kong

Date submitted: 15 Jan 2006 Electronic form version 1.4