Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

DFT study of the structural properties of silver halides: LDA vs GGA calculations.[1] G. MURRIETA, Facultad de Matematicas, UADY, Mexico, R. DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, L.A. PALOMINO-ROJAS, M. LOPEZ-FUENTES, G.H. COCOLETZI, N. TAKEUCHI, Instituto de Fisica, BUAP, Mexico — We perform total energy calculations to investigate the atomic structure of three silver halides: AgCl, AgBr, and AgI in the sodium chloride, cesium chloride, zincblende and wurtzite structures. Calculations are done within the density functional theory. We employ the full potential LAPW method, and the exchange-correlation potential energies are treated in the LDA and GGA approximations. We find that LDA correctly predict the ground state structure of all three binary compounds: rocksalt for AgCl and AgBr, and zincblende/wurtzite for AgI, while GGA always prefer the more covalent zincblende/wurtzite configurations. We observe that the distribution of electron densities for rocksalt is more homogeneous than for zincblende. As a consequence, the energy difference between zincblende/wurtzite and rock-salt phases is enhanced in the GGA approximation, predicting the wrong ground state structure for AgCl and AgBr. Assuming the right experimental structure, the GGA approximation gives lattice parameters, bulk moduli and cohesive energies closer to experimental values.

[1]Supported by CONACYT, SEP-PROMEP, and UNAM-DGAPA.

Romeo de Coss
Department of Applied Physics

Date submitted: 20 Nov 2006 Electronic form version 1.4