Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ab-initio Calculation of Zero-Field Spin Splitting in Heterostructures of III-V and II-VI Semiconductors. ATHANASIOS CHANTIS, MARK VAN SCHILFGAARDE, Arizona State University, VLADIMIR ANTROPOV, Ames Lab — We have developed a fully relativistic ab-initio transport method within the Linear Muffin Tin Orbitals (LMTO) Principal Layer Green Function framework. The calculated spin orbit induced band splittings of several III- V and II-IV bulk semiconductors are in excellent agreement with a well tested perturbative approach, as well as with previous fully relativistic results and available experimental data. The orbital magnetic moment of several 3d transition metals are also in excellent agreement with the perturbative approach and previous fully relativistic results. The method is used for a first principles investigation of Rashba and Dresselhaus effects in III-V and II-VI compounds asymmetric quantum wells, double barrier and single barrier heterostructures. The magnitude and ratio of the two effects determine the spin scattering ratio and anisotropy in quantum wells. These quantites are also important for the construction of spin modulators. With the present method periodic boundary conditions are not required; thus electric fields can be applied without the need for Berry phases. It is possible to obtain reliable values from first principles for a wide variety of geometries, and to clearly distinguish the Dresselhaus and Rashba contributions. The progress of the work and several results will be reported.

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Date submitted: 30 Nov 2004 Electronic form version 1.4