Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Rashba-type spin-orbit splitting in ultrathin Bi films G. BIHLMAYER, Inst. f. Festkoerperforschung, FZ Juelich, Germany, YU. M. KOROTEEV, Inst. of Strength Physics and Materials Science, Tomsk, Russia, E.V. CHULKOV, Donostia International Physics Center, San Sebastian, Spain, S. BLÜGEL, Inst. f. Festkoerperforschung, FZ Juelich, Germany — Due to their electronic similarity with graphene sheets, surfaces and thin films of the semimetal bismuth have recently received considerable interest. A systematic study of thin ($1-6$ bilayers) films in (111) and (110) orientation is presented, employing density functional theory calculations. Due to the different coordination of the surface atoms in these two cases, a large variation of the conducting properties of the films is found. The evolution of surface states is studied as a function of the film thickness and by comparison to thicker films and simulations of the semiinfinite crystals. Interesting features arise from the strong spin-orbit effects in Bi and the resulting Rashba-type spin-splitting of the surface states. The spin-polarization of these states changes as these states transform into quantum well states at the Brillouin zone boundary. The results are compared with recent experimental results on Bi films on Si substrates.

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Date submitted: 23 Nov 2007 Electronic form version 1.4