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Magneto-optical second-harmonic generation from a structurally optimized Fe/W(110) surface TORSTEN ANDERSEN, WOLFGANG HÜBNER, Condensed Matter Theory Group, Department of Physics, Kaiserslautern University of Technology, Box 3049, D-67653 Kaiserslautern, Germany — The nonlinear magneto-optical response from a structurally optimized W(110) surface with a magnetic Fe overlayer is calculated from first principles. The electronic structure of the ground state is calculated using the full-potential LAPW method with firstorder relativistic corrections, and the magneto-optical properties are obtained in the electric dipole approximation. We present results for the magnetic anisotropy energy as well as the nonlinear optical properties, including the susceptibility tensor, intensities in various optical configurations, angular dependences, and the nonlinear optical Kerr effect. We find that both the easy axis as well as the hard axis are in the surface plane, with the easy along the $1\overline{10}$ -direction and the hard axis along the 001-direction. We show how the direction of magnetization changes the magneto-optical properties.

Torsten Andersen Condensed Matter Theory Group, Department of Physics, Kaiserslautern University of Technology

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