Abstract Submitted
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Ab initio Calculation of optical properties of II-VI semiconductor surfaces[1] R.A. VAZQUEZ-NAVA, NORBERTO ARZATE, Centro de Investigaciones en Optica A. C., B.S. MENDOZA, Centro de Investigaciones en Optica — In this work we present some *ab initio* calculations of reflectance anisotropy spectra (RAS) of VI-II semiconductor surfaces having different surface reconstructions. We use an *ab initio* pseudopotential formalism in the framework of the density functional theory and within the local density approximation (DFT-LDA). We study the (001) polar surface of cadmium telluride (CdTe) and zinc telluride ZnTe with differents reconstructions. Also we obtain RAS using a microscopic formulation based on a semi-empirical tight binding (SETB) approach which includes spin-orbit (SO) interactions [1]. We show RAS of each surface reconstruction and compare both theoretical results with experimental results [2]. We find a good agreement between experimental and theoretical spectra.

[1] R.A. Vázquez-Nava, B.S. Mendoza and C. Castillo, Phys. Rev. B **70**, 165306 (2004).
[2] R. E. Balderas-Navarro, K. Hingerl, W. Hilber, D. Stifter, A. Bonanni and H. Sitter, J. Vac. Sci. Technol. B **18**, 2224 (2000).

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