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Record 1 of 1**Title:** Calculation of the Energy Band Diagram of a Photoelectrochemical Water Splitting Cell**Author(s):** Cendula, P (Cendula, Peter); Tilley, SD (Tilley, S. David); Gimenez, S (Gimenez, Sixto); Bisquert, J (Bisquert, Juan); Schmid, M (Schmid, Matthias); Gratzel, M (Gratzel, Michael); Schumachert, JO (Schumachert, Juergen O.)**Source:** JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 118 **Issue:** 51 **Pages:** 29599-29607 **DOI:** 10.1021/jp509719d **Published:** DEC 25 2014**Times Cited in Web of Science Core Collection:** 13**Total Times Cited:** 13**Usage Count (Last 180 days):** 10**Usage Count (Since 2013):** 70**Cited Reference Count:** 51**Abstract:** A physical model is presented for the semiconductor electrode of a photoelectrochemical cell. The model accounts for the potential drop in the Helmholtz layer and thus enables description of both band edge pinning and unpinning. The model is based on the continuity equations for charge carriers and direct charge transfer from the energy bands to the electrolyte. A quantitative calculation of the position of the energy bands and the variation of the quasi-Fermi levels in the semiconductor with respect to the water reduction and oxidation potentials are presented. Calculated photocurrent-voltage curves are compared with established analytical models and experimental data. Our model calculations are suitable to enhance understanding and improve the properties of semiconductors for photoelectrochemical water splitting.**Accession Number:** WOS:000347360200016**Language:** English**Document Type:** Article**KeyWords Plus:** SEMICONDUCTOR ELECTRODES; OXYGEN EVOLUTION; FILMS; CONVERSION; HEMATITE; SPECTROSCOPY; PHOTOANODES; CONDUCTION; KINETICS; LIGHT**Addresses:** [Cendula, Peter; Schmid, Matthias; Schumachert, Juergen O.] Zurich Univ Appl Sci ZHAW, Inst Computat Phys, CH-8401 Winterthur, Switzerland.

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