Abstract Submitted
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Opto-electronic properties of Ta_3N_5: a joint experimental and theoretical study[1] JULIANA MORBEC, Department of Chemistry, University of California, Davis, California 95616, USA, DARIO ROCCA, University of Lorraine, Nancy, France, BLAISE PINAUD, THOMAS JARAMILLO, Department of Chemical Engineering, Stanford University, 381 North-South Axis, Stanford, California 94305, USA, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago, Chicago, Illinois 60637, USA — Tantalum nitride (Ta_3N_5) is considered a promising material for use in photoelectrochemical cells, due to its suitable band gap for visible light absorption and favorable band-edge positions for water splitting. However, Ta_3N_5 films have been recently shown to exhibit low photocurrent (i.e. less than 50% of the theoretical limit). We report a joint experimental and ab initio theoretical study of the opto-electronic properties of Ta_3N_5, aimed at understanding possible reasons for the limited photocurrent. Our experimental optical spectra of films with different thicknesses show two absorption edges at 2.1 and 2.5 eV. To provide an interpretation of these features, we performed ab initio calculations, at several levels of theory, of the electronic band structure and optical absorption spectra of Ta_3N_5. We employed density functional theory with semi-local (PBE/LDA) and hybrid (PBE0/HSE06) functionals and many body perturbation theory at the G_0W_0 level, and we obtained optical spectra by solving the Bethe-Salpeter equation within density matrix perturbation theory.

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