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Electronic and optical properties of TiN_x from first-principles calculations FAISAL MEHMOOD, RUTH PACHTER, Air Force Research Laboratory, Materials & Manufacturing Directorate, Wright-Patterson Air Force Base, Ohio 45433 — We present a systematic study of the structural, electronic and optical properties of bulk phases of TiN_x and its (111) surface for mimicking thin films, which are of interest technological in applications such as coatings. Time-dependent density functional theory and the GW approximation have been applied. In the first stage, a comparison between experimental ellipsometry data and the calculated optical absorption spectra, for example, for a surface upon changing stoichiometry, has been undertaken. The results demonstrate applicability of the methods in prediction of optical excitations for titanium nitride thin film, deposited with varying nitrogen flow rates.

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