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Oxides – a challenge for (theoretical) spectroscopy P. RINKE, H. JIANG, M. SCHEFFLER, Fritz-Haber-Institut der MPG, 14195 Berlin, A. GREULING, M. ROHLFING, Universitaet Osnabrueck, 49069 Osnabrueck, A. JANOTTI, E. KIOUPAKIS, C. G. VAN DE WALLE, University of California at Santa Barbara, CA 93106 — Oxides are of tremendous technological importance, yet challenging materials to characterize. In many cases the agreement between experimental and theoretical spectroscopy observed for other material classes has not been attained. We use rutile TiO_2 as an example to illustrate some of the problems. Many-body perturbation theory in the G_0W_0 approach based on density-functional theory in the local-density approximation gives a fundamental band gap of 3.3 eV in seemingly good agreement with the 3.3 ± 0.5 eV measured in direct and inverse photoemission [1]. However, the lowest exciton computed in Bethe-Salpeter calculations for the optical spectrum is found at an energy of 3.21 eV, while optical experiments only give 3.03 eV [2]. Polaronic effects, i.e. the renormalization of the band edges due to electron-phonon coupling, reduce the band gap, but it remains a challenge to include the ionic contribution to the dielectric function, which can be substantial in oxides, in the G_0W_0 calculations and to incorporate both effects consistently into Bethe-Salpeter calculations. Another aspect to consider is the role of electron correlations. [1] Y. Tezuka *et al.*, J. Phys. Soc. Jpn. **63**, 347 (1994). [2] J. Pascual *et al.*, Phys. Rev. B **18**, 5606 (1978).

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