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Quasiparticle electronic structure calculations of F centers in SrTiO₃ perovskite CHANDRIMA MITRA, ALEX DEMKOV, University of Texas at Austin — Among the broad class of oxides, ABO₃ perovskites have attracted a lot of attention in the recent past due to its beneficial material properties. SrTiO₃ is one such example of this class of compounds. It shows a wide range of properties from being ferroelectric to exhibiting superconducting properties in doped SrTiO₃. The anomalous dielectric properties in this material make it a potential candidate for technological applications. However, being a semicovalent oxide, the complexities in its electronic structure have hindered a proper characterization of the system. For instance, the intrinsic excitonic luminescence, in this system, is not well understood and there is no general agreement as to whether it is caused by defects or due to self trapped excitons. This calls for an accurate theoretical description of the electronic levels as well as the various defect states in this material. In this work we present results for quasiparticle GW calculations of pure as well as *defective* SrTiO₃ containing oxygen vacancies which form F centers in these compounds. From a quasiparticle description of the system excitonic properties of SrTiO₃ will be examined.

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