Abstract Submitted
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All-electron GW quasiparticle band structures of group 14 nitride compounds[1] IEK-HENG CHU, Department of Physics and the Quantum Theory Project, University of Florida, Gainesville, Florida, USA, ANTON KOZHENIKOV, THOMAS SCHULTHESS, Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland, HAI-PING CHENG, Department of Physics and the Quantum Theory Project, University of Florida, Gainesville, Florida, USA — We have investigated the group 14 nitrides (M_3N_4) in both the spinel phase (with M=C, Si, Ge and Sn) and the beta phase (with M=Si, Ge and Sn) using density functional theory (DFT) with the local density approximation (LDA). The Kohn-Sham energies of these systems are first calculated within the framework of full-potential LAPW and then corrected using single-shot G_0W_0 calculations, which we have implemented in the Exciting-Plus code. Direct bands gap at the Γ point are found for all spinel-type nitrides. The calculated band gaps of Si_3N_4, Ge_3N_4 and Sn_3N_4 agree with experiment. We also find that for all systems studied, our GW calculations with and without the plasmon-pole approximation give very similar results, even when the system contains semi-core 3d electrons. These spinel-type nitrides are novel materials for potential optoelectronic applications.

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