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Physical properties of the wide band gap II-IV nitride MgSiN₂ MIKAEL RÅSANDER, JAMES QUIRK, MICHELLE MORAM, Imperial College London — The Group II-IV nitride semiconductors are emerging as promising alternatives to III-nitrides in ultraviolet LED applications. These materials have wurtzite-derived orthorhombic crystal structures and can be obtained by substituting pairs of Group III atoms in a III-nitride for a single Group II atom and a single Group IV atom. Here we will focus on MgSiN₂, which is the equivalent II-IV nitride to wurtzite AlN. A detailed comparison of the properties obtained by first principles calculations and experiment of these two systems will be performed. It will be shown that MgSiN₂ has a large indirect band gap of similar size to the direct band gap of AlN, while having a crystal size which is intermediate between AlN and GaN.¹ MgSiN₂ should therefore facilitate better lattice matching during film growth compared to AlN, and therefore constitutes a good candidate material to be used in novel high efficiency UV-LEDs.

¹J. B. Quirk, M. Råsander, C. M. McGilvery, R. Palgrave and M. A. Moram, Appl. Phys. Lett. 105, 112108 (2014), M. Råsander and M. A. Moram, Mater. Res. Express 3, 85902 (2016).

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