Doping effects on the electronic and magnetic properties of V$_2$O$_5$\

CHURNA BHANDARI, WALTER R.L. LAMBRECHT, Case Western Reserve University — We study doping of the V$_2$O$_5$ split-off conduction band using different methods: by adding electrons compensated by an artificial homogeneous background, a virtual crystal approximation (VCA), by changing the atomic number $Z_v$ and explicitly by intercalating Na as a dopant. The former two are mathematical models to simulate injected charge by gating, the latter occurs in the vanadium bronze NaV$_2$O$_5$. We also study Na$_{1-x}$V$_2$O$_5$ using the VCA by changing $10 \leq Z_{Na} \leq 11$. We discuss the electronic band structure and the optical conductivity using the quasiparticle self-consistent QSGW method including a lattice polarization effect and the local density functional method with Hubbard-$U$ correction (LSDA+$U$) for all these models. We show that the ground state prefers anti-ferromagnetic order along the chain (crystallographic $b$) direction and extract various near neighbor exchange interactions from total energy differences of different spin configurations. We find that the coupling between the nearest V-neighbors changes from anti-ferromagnetic to ferromagnetic when the electron concentration is reduced from half filling of the band (1e/V atom) to about 0.88 e/V atom. The magnetic moment gradually decreases with decreasing electron concentration.

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