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Doping effects on the electronic and magnetic properties of V_2O_5[1]

CHURNA BHANDARI, WALTER R.L. LAMBRECHT, Case Western Reserve University — We study doping of the V_2O_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_2O_5. We also study $Na_{1-x}V_2O_5$ 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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