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Photoemission and Inverse Photoemission Spectra of Doped Mott Insulators with Orbital Degeneracy [1]

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We analyze electron localization induced by random charged defects in the vanadium $R_{1-x}\mathrm{Ca}_x\mathrm{VO}_3$ perovskites (R=La,,Y). Using the inverse participation number we explore the degree of localization and the doping dependence for all electron states in the spectrum. Random charged defects yield a robust insulating state in the spin-orbital ordered system. The soft gap in the defect states inside the Mott-Hubbard gap is triggered by a combination of e-e interactions and a kinetic mechanism [1]. We show that doped holes bound near the charge defects delocalize over active bonds, controlled by the spin-orbital structure, which in turn determine the reduction of spin- and orbital order. We discuss the novel structures arising in photoemission and the inverse participation number of different states.

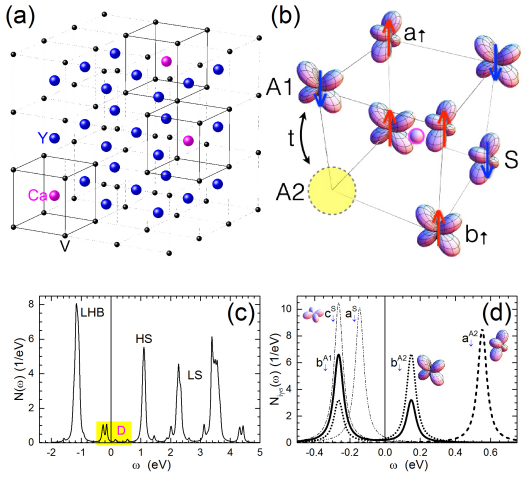

Figure 1: Random Ca defects (pink circles) in $\mathrm{Y}_{1-x}\mathrm{Ca}_x\mathrm{VO}_3$ lattice (a) generate one hole (yellow circle) at each cube around the defect, confined to an active $\langle$A1,A2$\rangle$ bond (b). Occupied t_{2g} orbitals $\{yz, zx\}$ alternate in G-type order, coexisting with C-type antiferromagnetic order of $S = 1$ spins. (c) Within the Mott-Hubbard gap the defect states D separate lower Hubbard band (LHB) and the high-spin/low-spin (HS/LS) states of the upper Hubbard band, forming a smaller kinetic gap (d). The figure is reproduced from [2].

[1] A. Avella, P. Horsch, and A. M. Oleś, Phys. Rev. B **87**, 045132 (2013).
[2] A. Avella, A. M. Oleś, and P. Horsch, Phys. Rev. Lett. **115**, 206403 (2015).

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