Since the discoveries of high-temperature superconductivity and colossal magnetoresistance in Mott insulators made metallic by hole-doping, 3d transition metal oxides have remained at the forefront of research. Their many lattice and electronic (orbital, charge, and spin) degrees of freedom are coupled by effective interactions (electron-phonon, hopping, t, Coulomb repulsion, U, and Hunds rule coupling, J), and when some of these are of similar magnitude, competing phases may exist in the region of controllable compositions, fields, and temperatures. The interactions tend to remove low-energy degrees of freedom, e.g., to reduce the metallicity. This rarely happens by merely shifting spectral weight from a quasiparticle band into incoherent Hubbard bands, as in the U/t-driven metal-insulator transition for the single-band Hubbard model, but is usually assisted by lattice distortions which break the degeneracy of low-energy orbitals and split the corresponding quasiparticle – or partly incoherent – bands away from the chemical potential.

When going from 3d to 4d transition metal oxides, the larger extent of the 4d orbitals cause the hopping, t, and the coupling to the lattice to increase, and U and J to decrease. It was therefore hardly surprising that the Fermi surface (FS) of Sr$_2$RuO$_4$ measured by various techniques like dHvA and ARPES was in good agreement with LDA calculations, in which strong electronic correlations are only moderately represented. It was, however, surprising that substituting Rh for Ru, e.g. adding one electron and one nuclear charge and roughly keeping the crystal structure, lead to strong disagreement between experiments and LDA theory [1].

In both the ruthenates and the rhodenates the Fermi level crosses the t$_{2g}$ manifold, but in the latter, the interaction between the xy and the x$^2$-y$^2$ orbitals due to the rotation of the RhO$_6$ octahedra around the z-axes is such as to gap those two bands at the Fermi level. As a consequence, only the equivalent 1D xz- and yz-bands, which hardly hybridize with the other d-bands nor with each other, remain at the Fermi level, with the single t$_{2g}$ hole distributed equally between them. However, also the LDA FS calculated for the proper structure deviates substantially from the experimental FS [1,2]. This discrepancy clearly seen in Fig.1 (LDA) is disturbing because there is no experimental indication of any further distortion. Hence, Coulomb-enhanced crystal-field splitting can not be the solution to this puzzle.

In order to resolve this puzzle we first fitted the Fermi surface to a tight binding model consisting of the xz- and yz-orbitals on a 2D square lattice, e.g., neglecting the rotation of the RhO$_6$ octahedra and the hopping in the z-direction [3]. The resulting bands and Fermi surfaces with and without spin-orbit (SO) coupling are shown in Figs. 2 and 3 respectively. The perfect fit was obtained with the parameters in the figure caption.
We then performed \textit{ab initio} LDA calculations including the SO coupling \cite{3,4} and later also the on-site Coulomb effects in the LDA+\textit{U} approximation. The results are shown in Fig. 1. As may be seen in Fig. 1 (LDA+SO), the agreement with ARPES is less good for the \textit{ab initio} relativistic LDA FS: the SO splitting along $\Gamma M$ is too small. In fact, fitting the LDA+SO FS to our tight-binding model, yields essentially the same values for $t_\pi/\varepsilon_F$ and $t_\delta/\varepsilon_F$, but the SO-parameter $\zeta/\varepsilon_F$ is smaller than $\zeta_{\text{ARPES}}/\varepsilon_F$ by the large factor of 2.15. The LDA+SO calculation yields: $\zeta=0.13\,\text{eV}$, a value which is smaller than the 0.16\,eV obtained for elemental fcc Rh due to the $O p_z$ tails of the rhodate Wannier orbitals.

The TB results in Figs. 2 and 3 are obtained with $\zeta=0$.

In conclusion, resolution of the Sr$_2$RhO$_4$ puzzle has taught us that although usually neglected in 4d-oxides, the spin-orbit coupling belongs to the list of competing interactions which cause the rich physics of these materials.

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