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**How Cation-Covalency controls Electron Localization in t2g Perovskites** OLE KROGH ANDERSEN, ATSUSHI YAMASAKI, Max-Planck Institute FKF, Stuttgart, EVA PAVARINI, Forschungszentrum Juelich — In the series of perovskites, SrVO<sub>3</sub>-CaVO<sub>3</sub>-LaTiO<sub>3</sub>-YTiO<sub>3</sub>, the transition-metal d electron becomes increasingly localized and undergoes a Mott transition. By defining a low-energy Hubbard Hamiltonian in the basis of NMTO Wannier functions for the t<sub>2g</sub> LDA band and solving it in the single-site dynamical mean-field approximation, it was recently shown [1] that simultaneously with the Mott transition, the orbital fluctuations are strongly suppressed. Here, we explain the underlying chemical mechanisms [2]: Proceeding through the series, covalency between the empty large-cation-d states and the occupied oxygen-p states causes the oxygen octahedra to rotate and tilt. Moreover, since those oxygen-p orbitals which bond to the cations are the same as those which bond to the transition-metal t<sub>2g</sub> orbitals, the t<sub>2g</sub> Wannier functions exhibit residual covalency. This splits the t<sub>2g</sub> levels and reduces the width of the lowest subband. Cation covalency thus causes the electron to localize in LaTiO<sub>3</sub> and YTiO<sub>3</sub>. [1] E. Pavarini, S. Biermann, A. Poteryaev, A.I. Lichtenstein, A. Georges, O.K. Andersen, Phys. Rev. Lett. 92 (2004) 176403. [2] E. Pavarini, A. Yamasaki, J. Nuss, O.K. Andersen, New Journal of Physics 7 (2005) 188

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