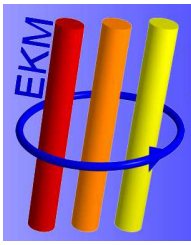


Elektronische Korrelationen und Magnetismus
Universität Augsburg

Computation of photoemission spectra of the doped Mott insulator $La_{1-x}Sr_xTiO_3$ using LDA+DMFT(QMC)

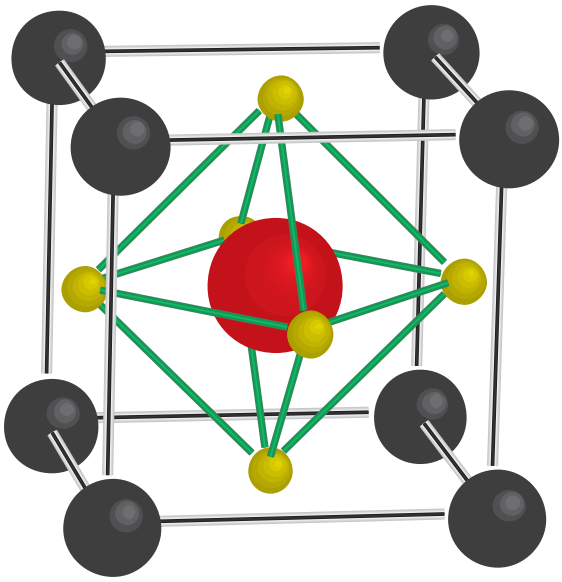
N. Blümer, I.A. Nekrasov, K. Held, A.I. Poteryaev,
V.I. Anisimov, and D. Vollhardt

Eur. Phys. J. B **18**, 55 (2000); cond-mat/0010395

Outline

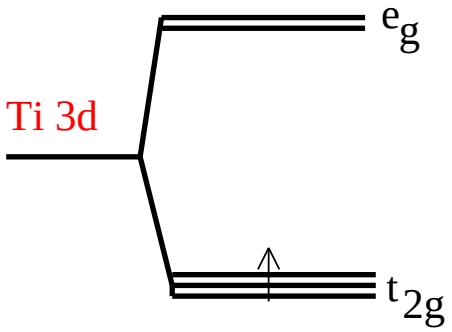
Introduction:	Structure of $La_{1-x}Sr_xTiO_3$; experimental PES
Theory:	DFT(LDA); extensions for strong correlations dynamical mean-field theory (DMFT) quantum Monte Carlo (QMC)
Results:	t_{2g} density of states; theoretical PES

Introduction



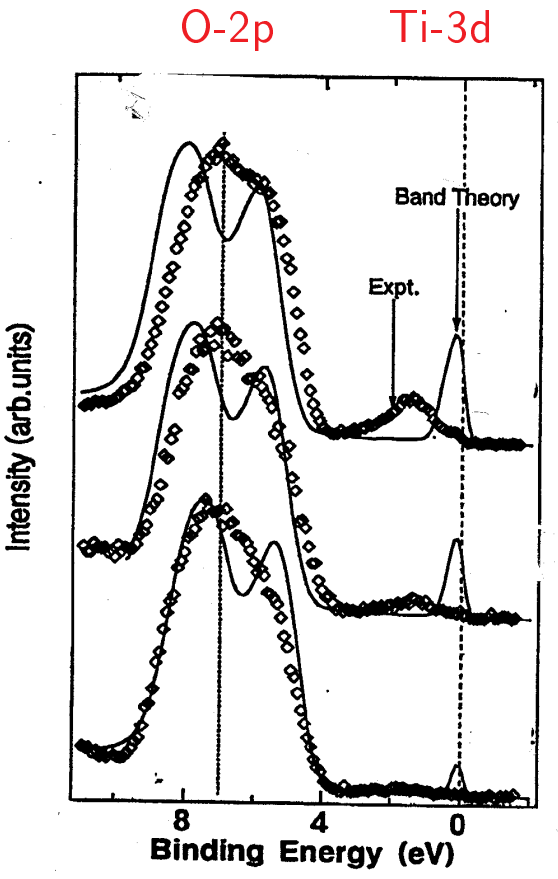
$La_{1-x}Sr_xTiO_3$

- La, Sr
- Ti
- O



Cubic Perowskite
slight orthorombic distortion

$x = 0$	$LaTiO_3$: AF insulator for $T < T_N = 125K$
$x > 0.05$	strongly correlated paramagnetic metal
$x = 1$	$SrTiO_3$: band insulator



[Fujimori et al., PRB **46**, 9841 (1992)]

photoemission spectra (PES)

- LDA fails when correlations become strong
- $La_{1-x}Sr_xTiO_3$ ($x \ll 1$) is typical strongly correlated transition metal oxide

Theory

	DFT/LDA		Model Hamiltonians
+	material specific: "ab initio"	−	input parameters unknown
−	fails for strong correlations	+	systematic many-body approach
+	fast code packages	−	computationally expensive

Density functional theory (Hohenberg-Kohn, Levy): $E_0 = E_0[\rho]$

$$E[\rho] = E_{\rm kin}[\rho] + E_{\rm ion}[\rho] + E_{\rm Hartree}[\rho] + E_{\rm xc}[\rho]$$

local density approximation (LDA): $E_{xc}[\rho] \rightarrow \int d^3r\ E_{xc}^{\rm jellium}(\rho(\mathbf{r}))$

interprete Kohn-Sham Lagrange parameters as single-particle energies
use localized basis (linear muffin tin orbitals, LMTO)
$\longrightarrow$ tight-binding Hamiltonian

$$\hat{H}^{\rm LMTO} = \sum_{ilm,jl'm',\sigma} \left(t_{ilm,jl'm'} \hat{c}^\dagger_{ilm,\sigma} \hat{c}_{jl'm',\sigma} + \varepsilon_{ilm} \hat{n}_{ilm,\sigma} \delta_{ilm,jl'm'} \right)$$

LDA+U: introduces Hubbard U for localized orbitals ($l = l_d$, treatment in static mean-field theory) [Anisimov, Zaanen, Andersen, PRB. **44**, 943 (1991)]

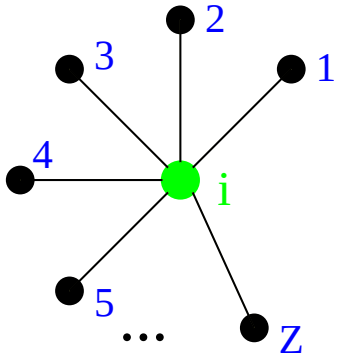
here: many-body approach

$$\hat{H} = \hat{H}^{\rm LMTO} + \frac{1}{2} \sum_{m\sigma \neq m'\sigma'} U_{mm'}\, \hat{n}^\sigma_m \hat{n}^{\sigma'}_{m'} - \frac{1}{2} U n_d (n_d - 1)$$

Approximation needed for treatment of $\hat{H}_{\rm corr}$:

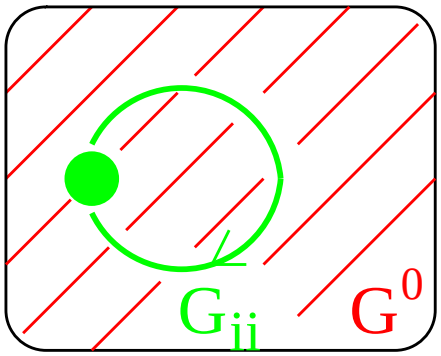
DMFT: Anisimov, Poteryaev, Korotin, Anokhin, Kotliar, J. Phys. **9**, 7359 (1997)
FLEX: Lichtenstein, Katsnelson, PRB **57**, 6884 (1998) (also Hubbard-I, DMFT)
Drchal, Janiš, Kudrnovský, PRB **60**, 15664 (1999)

LDA + DMFT



DMFT $\longrightarrow$

exact for $Z \to \infty$



lattice problem

single impurity Anderson model
+ self consistency condition

Metzner, Vollhardt, PRL **62**, 324 (1989); Georges et al., RMP **44**, 187 (1995)

For weak hybridization of t_{2g} orbital, orbital/spin-degenerate case:

$$G(z) = G^0(z - \Sigma(z)) = \int d\varepsilon \frac{\rho_0^{\mathrm{LMTO}}(\varepsilon)}{z - \Sigma(z) - \varepsilon}$$

$$G_{\nu m\sigma} = -\langle \psi_{\nu m\sigma} \psi^*_{\nu m\sigma} \rangle_{\mathcal{A}\{\psi,\psi^*;G^{-1}+\Sigma\}}; \quad z \to \omega_\nu = \frac{(2\nu+1)\pi}{\beta}$$

Numerical solution of LDA+DMFT(X)

IPT	Anisimov, Poteryaev, Korotin, Anokhin, Kotliar, J. Phys. **9**, 7359 (1997)
NCA	Zölfl, Pruschke, Keller, Poteryaev, Nekrasov, Anisimov, PRB **61**, 12810 (2000)
QMC	Katsnelson, Lichtenstein, PRB **61**, 8906 (2000)
	Liebsch, Lichtenstein, PRL **84**, 1591 (2000)

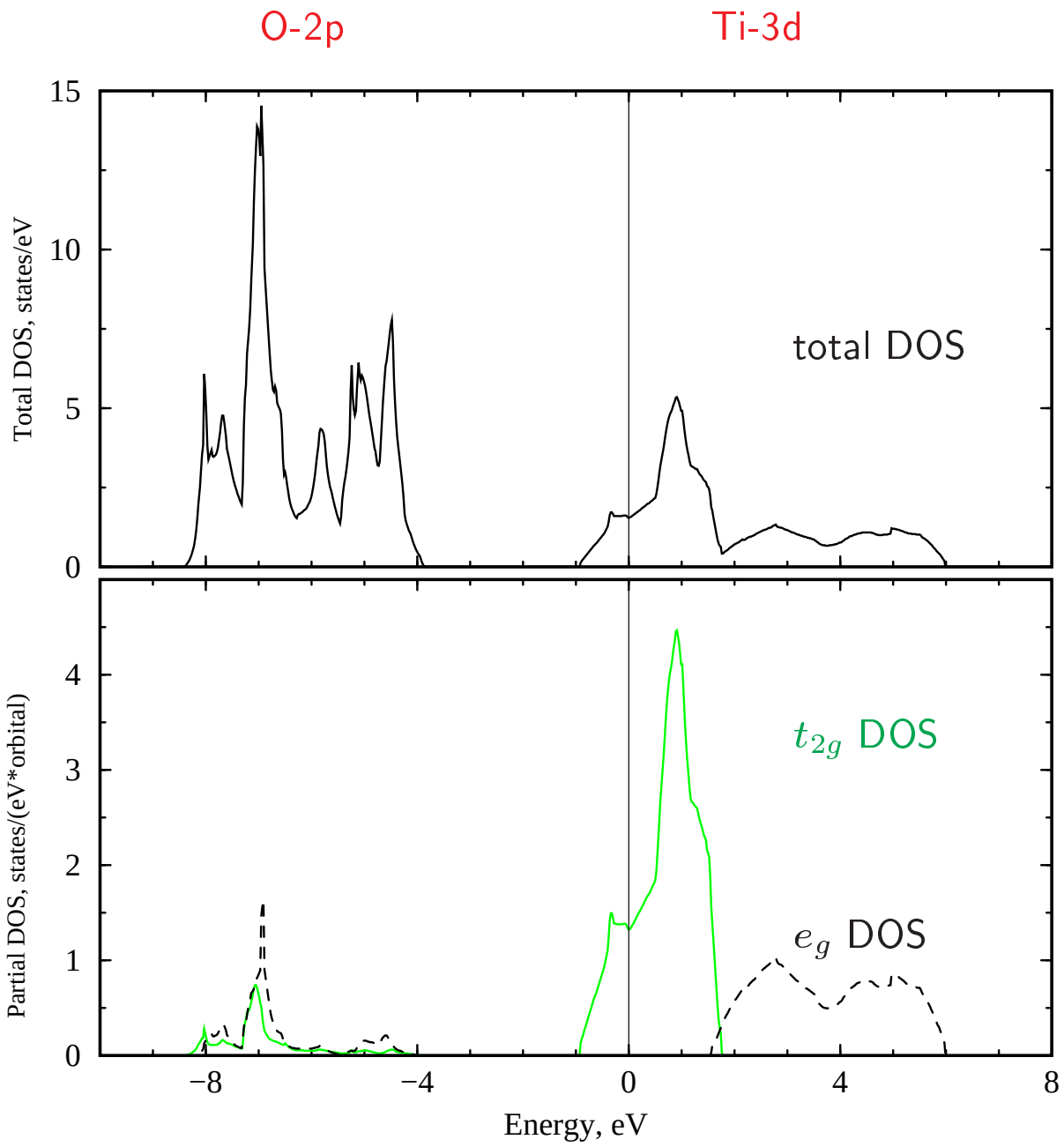
QMC solution of impurity problem (M interacting orbitals):

- discretization $\Delta\tau$ of imaginary time $\beta = \Lambda\Delta\tau$ $(\beta = 1/T)$
- discrete Hubbard-Stratonovich transformation
  $\to 2^{M(2M-1)\Lambda}$ different non-interacting systems
- MC importance sampling; computational cost $\propto M(2M-1)\beta^3$

Hirsch and Fye, PRL **56**, 2521 (1986)

Results

LDA-LMTO(ASA) calculation for $LaTiO_3$

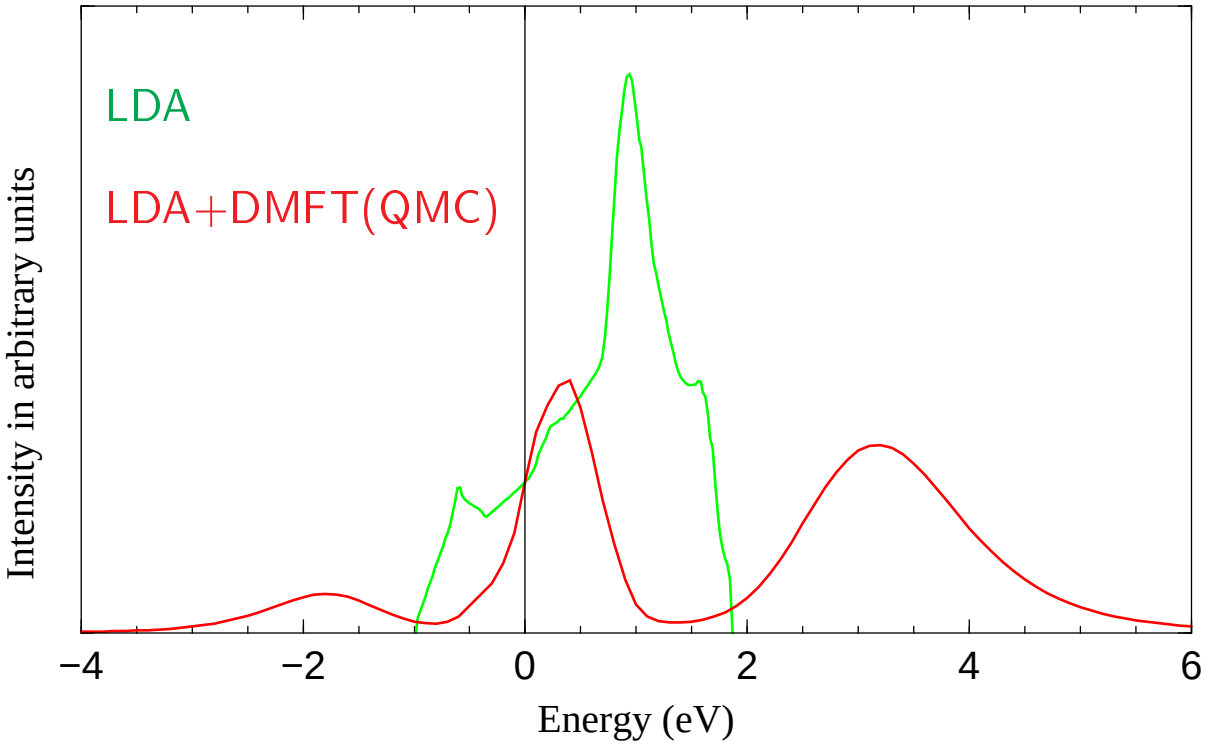


Orthorhombic structure approximated by cubic structure with same volume
$\longrightarrow$ slight overestimation of effective bandwidth

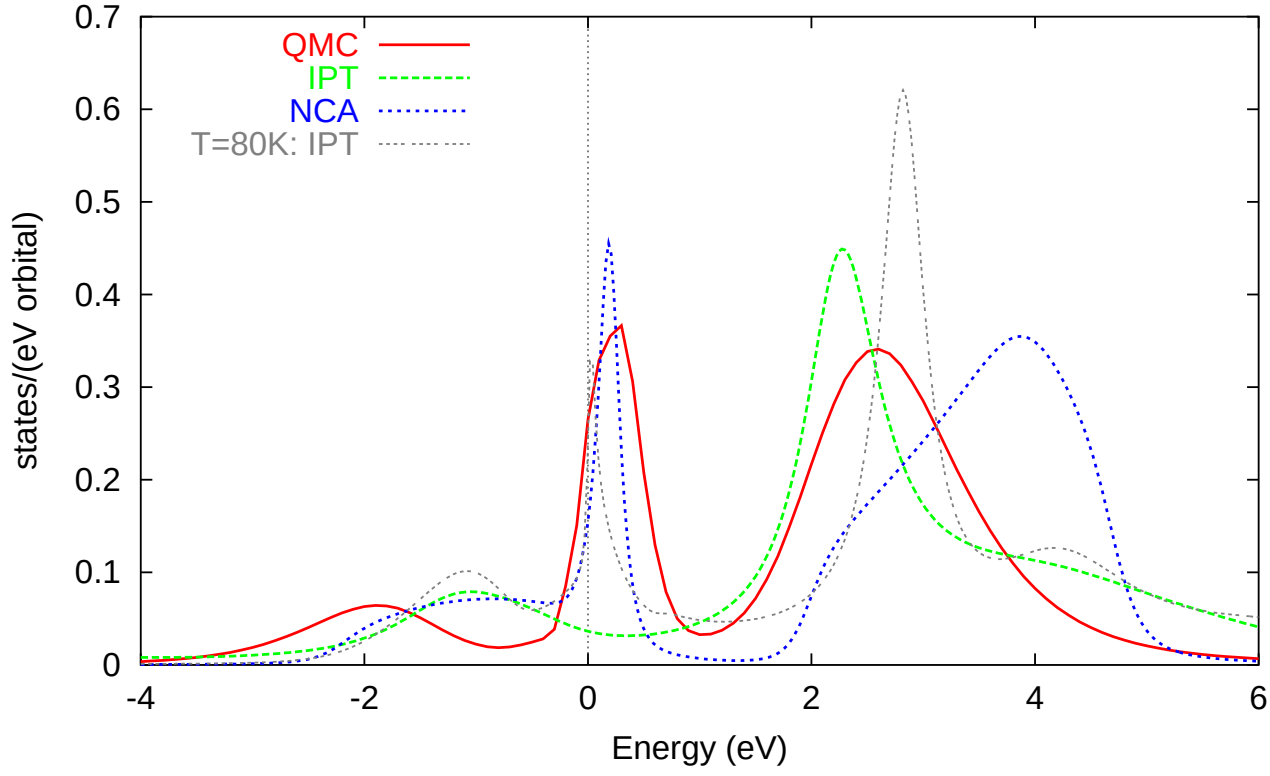
constrained LDA $\longrightarrow U_d \approx 3 - 5$ eV

DMFT calculation for $La_{1-x}Sr_xTiO_3$: partial t_{2g} DOS

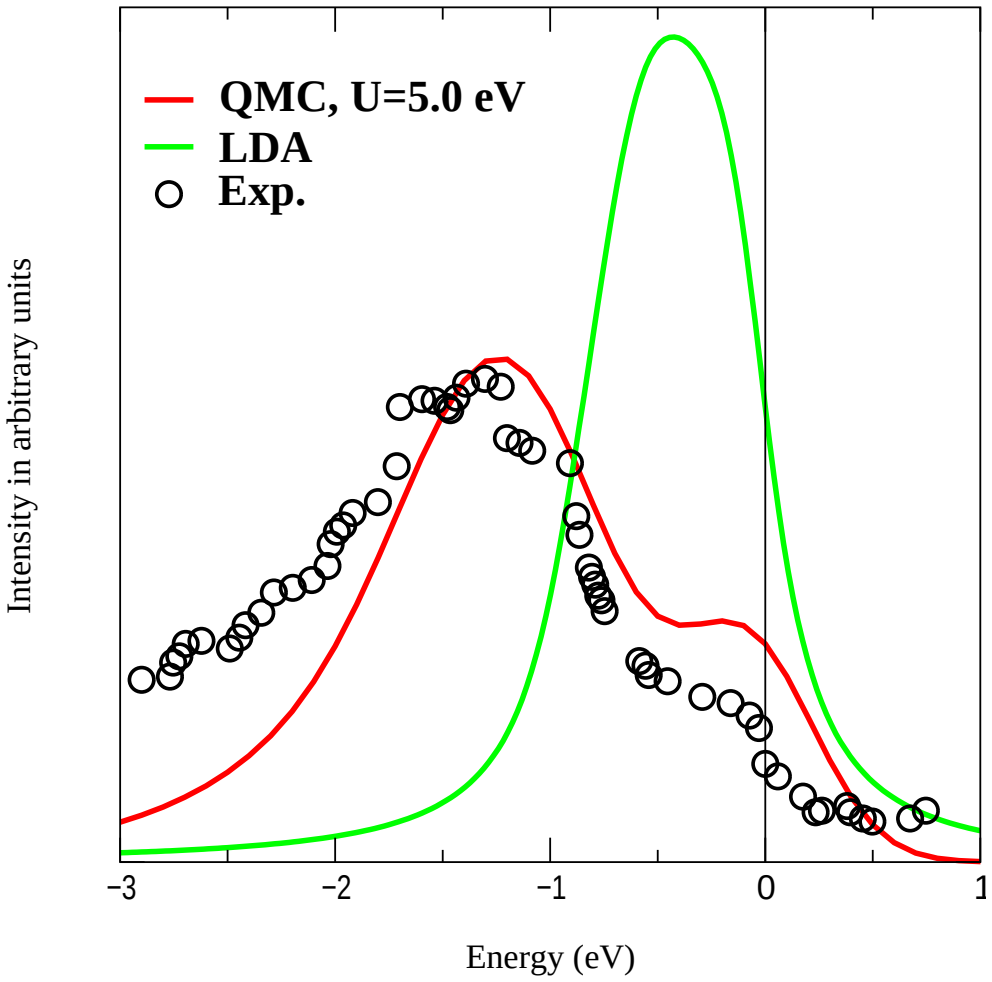
$x = 0.06$, $U = 4.0$ eV, $T = 0.1$ eV ~ 1000K, 3 degenerate bands



Comparison to approximate DMFT methods



Comparison with experiment: photoemission spectra (PES)



Experiment: Fujimori et al., PRL **69**, 1796 (1992)
Theory: DOS multiplied with Fermi step function; broadening 0.3 eV

Conclusion

- LDA + DMFT(QMC) yields qualitatively correct picture
- significant improvement over LDA
- QMC solution of DMFT superior to NCA, IPT

- include more orbitals, Hund's rule couplings
- other materials: V_2O_3 (see TT 6.13; Held et al., cond-mat/0011518)

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