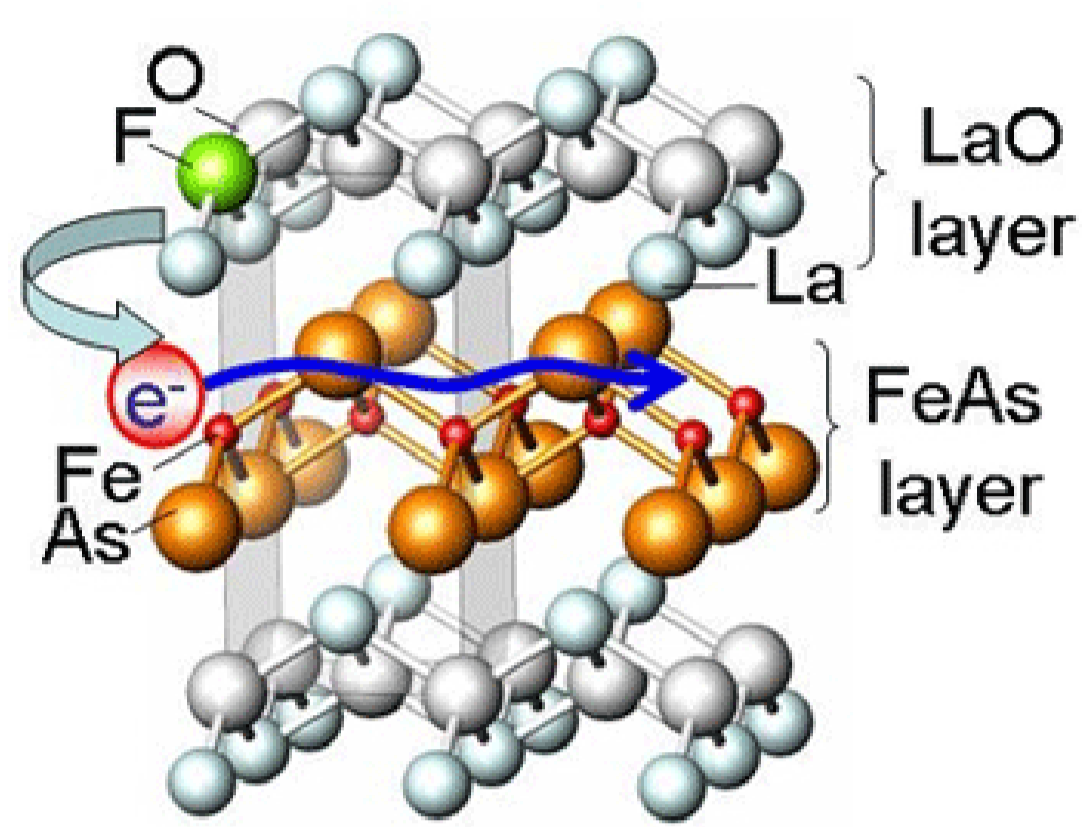


Pnictide Superconductors



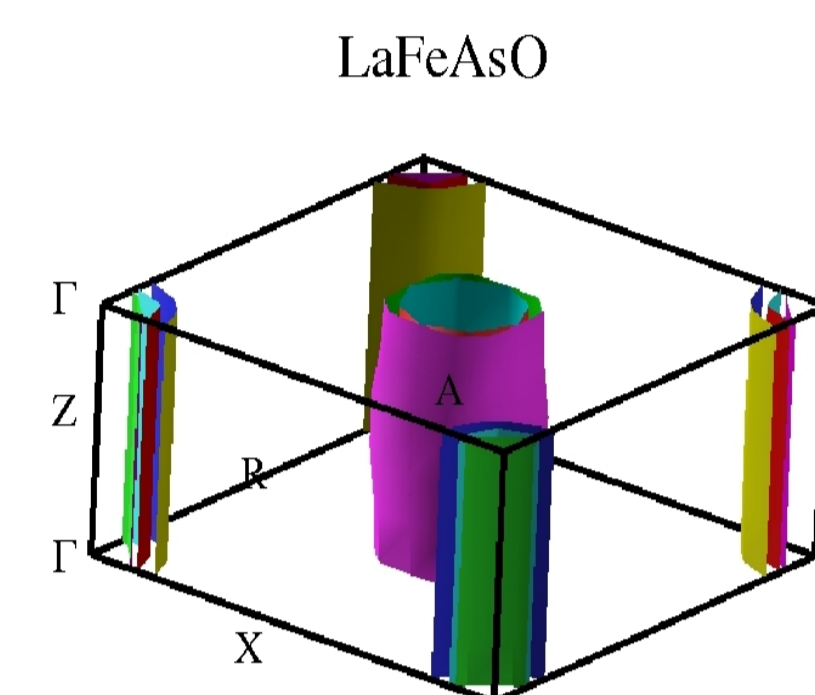
[J. Phys. Soc. J. 77 (2008) 053709]

Several families: 1111: e.g. LaOFeAs
122: e.g. BaFe₂As₂
11: e.g. Fe_{1+x}Se

'High' T_c of about 55 K (SmOFeAs doped)

Layered structure
charge transfer from LaO
layer to FeAs layer

low-energy bands: Fe-3d
Multiorbital physics!



Is the 3d band in FeAs superconductors as strongly correlated as in the cuprates?

Early calculations: From strongly correlated to very weakly correlated!

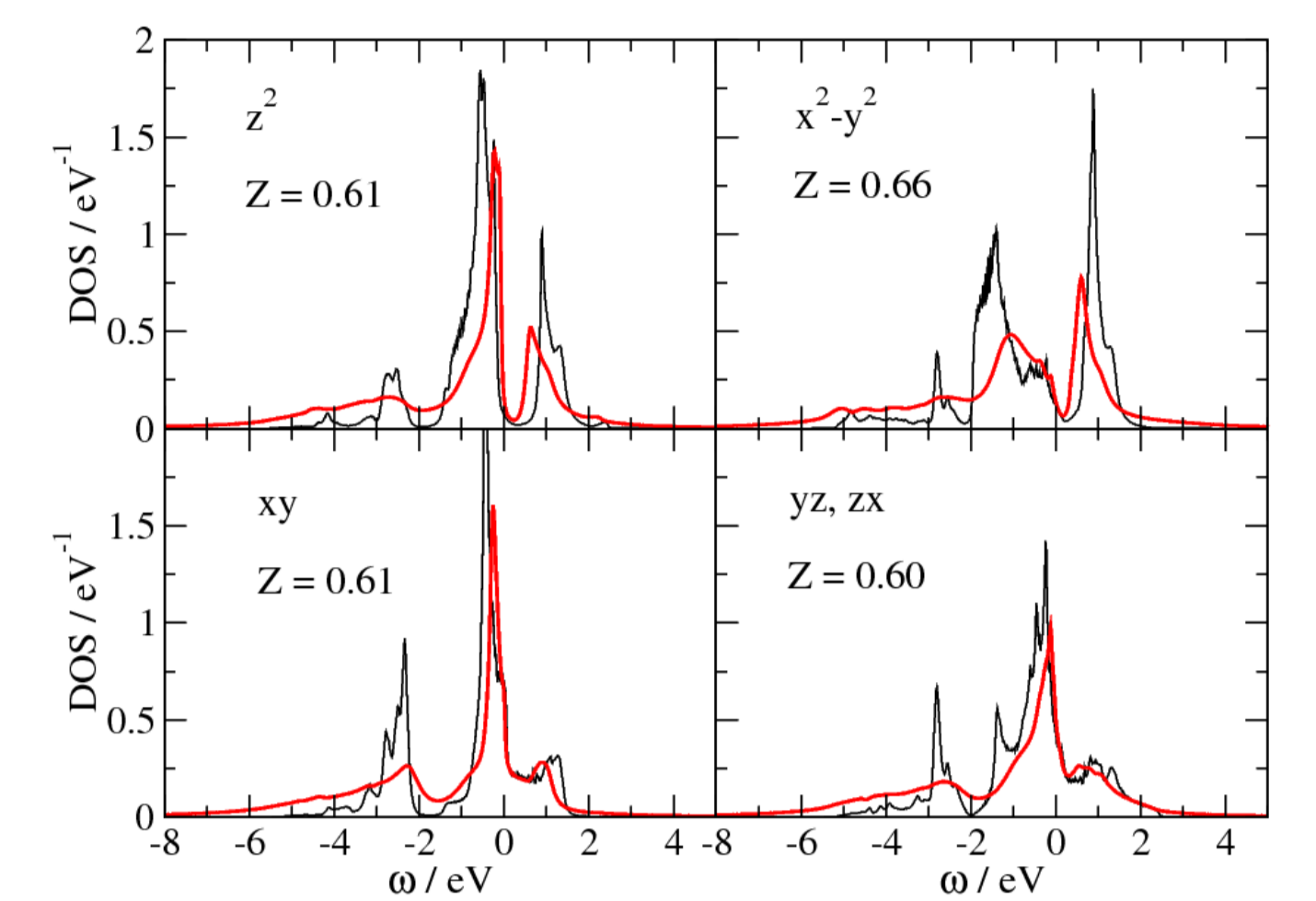
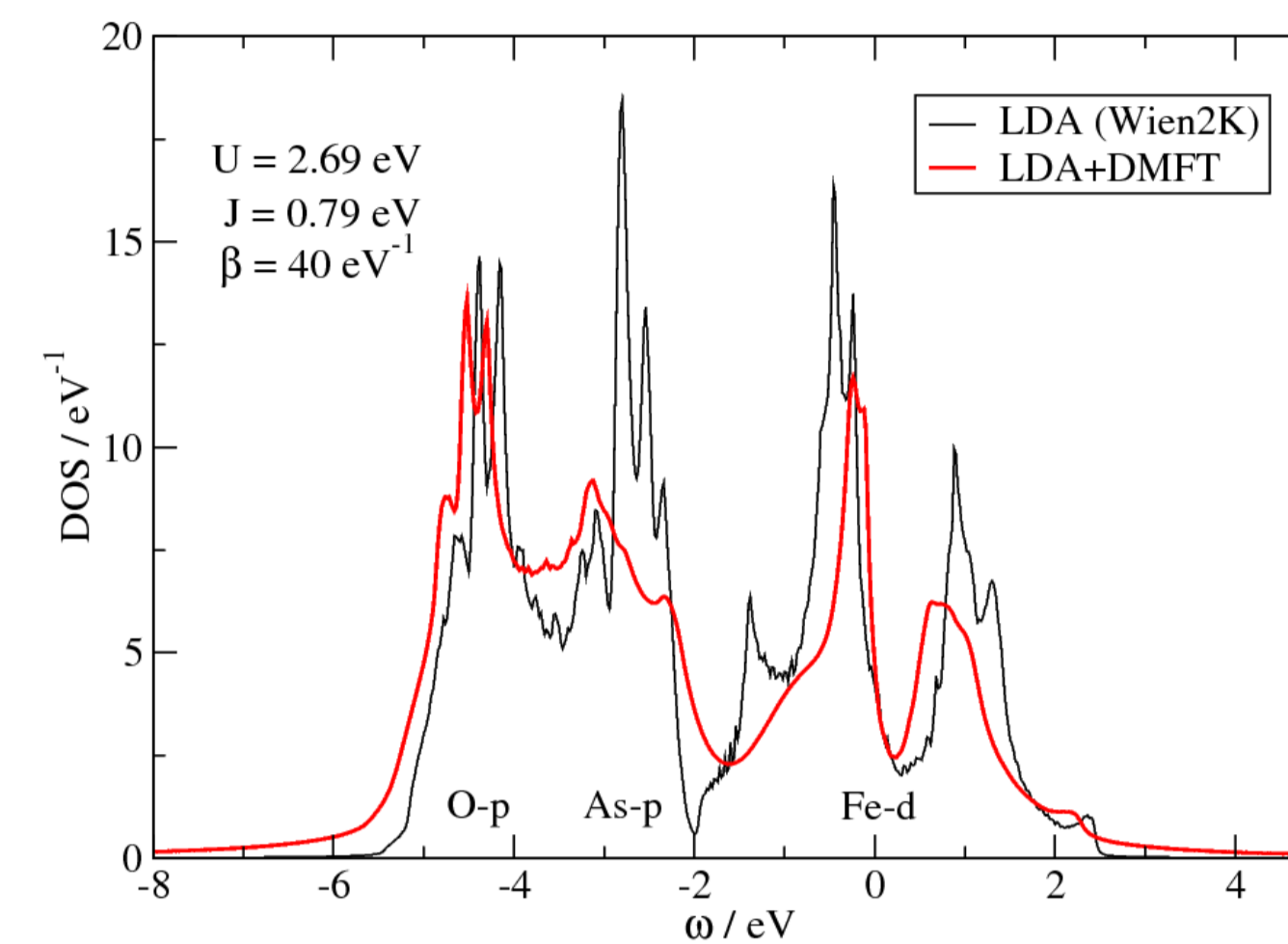
e.g. K. Haule et al.: On the verge of a Mott transition ($Z=0.1$) *PRL* **100**, 226402 (2008)

e.g. V. Anisimov et al.: Weakly correlated ($Z=0.5$) *Journal of Phys.:Condens. Mat.* **21**, 075602 (2009)

BUT: Similar methods, similar systems, similar parameters

**What is the reason of these inconsistencies?
How correlated is LaOFeAs?**

Density of states, Quasi-particle renormalization



dpp-hamiltonian: $W = [-5.5, 2.5]$ eV
Fe-d, As-p, O-p

$U_{av} = 2.79$ eV $J = 0.79$ eV from cRPA

Fe-d bands renormalized, As-p affected by correlations
O-p almost unchanged.

All orbitals show similar renormalization:
average $Z = 0.62$, effective mass $m^* = 1.62$

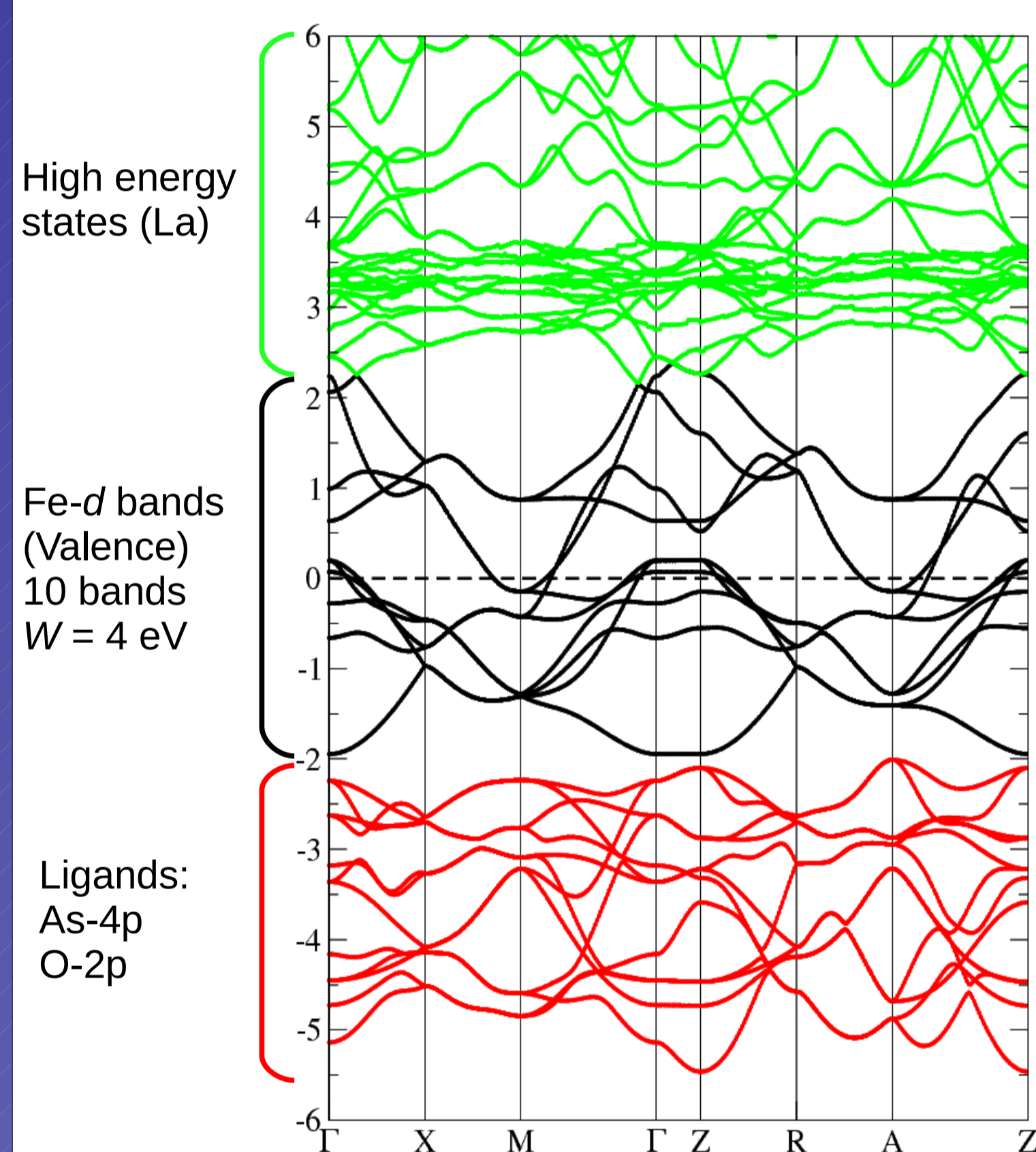
No indication for upper or lower Hubbard bands!

Experimentally: Mass renormalization of $m^* = 1.8 - 2.2$

Difference: Neglect of SDW state, no spatial spin fluctuations in single site DMFT

Note: DMFT Spectra at $\omega = 0$ coincide with LDA DOS \rightarrow Fermi liquid

LDA band structure for LaFeAsO



Correlated orbitals

Wannier functions constructed by **Projection**

$$|\tilde{\chi}_{km}^{\alpha,\sigma}\rangle = \sum_{\nu \in \mathcal{W}} \langle \psi_{k\nu}^{\sigma} | \chi_m^{\alpha,\sigma} \rangle |\psi_{k\nu}^{\sigma}\rangle$$

loc. orbital Bloch band

Orthonormalization

$$|w_{km}^{\alpha,\sigma}\rangle = \sum_{\alpha', m'} S_{m, m'}^{\alpha, \alpha'} |\tilde{\chi}_{km'}^{\alpha', \sigma}\rangle$$

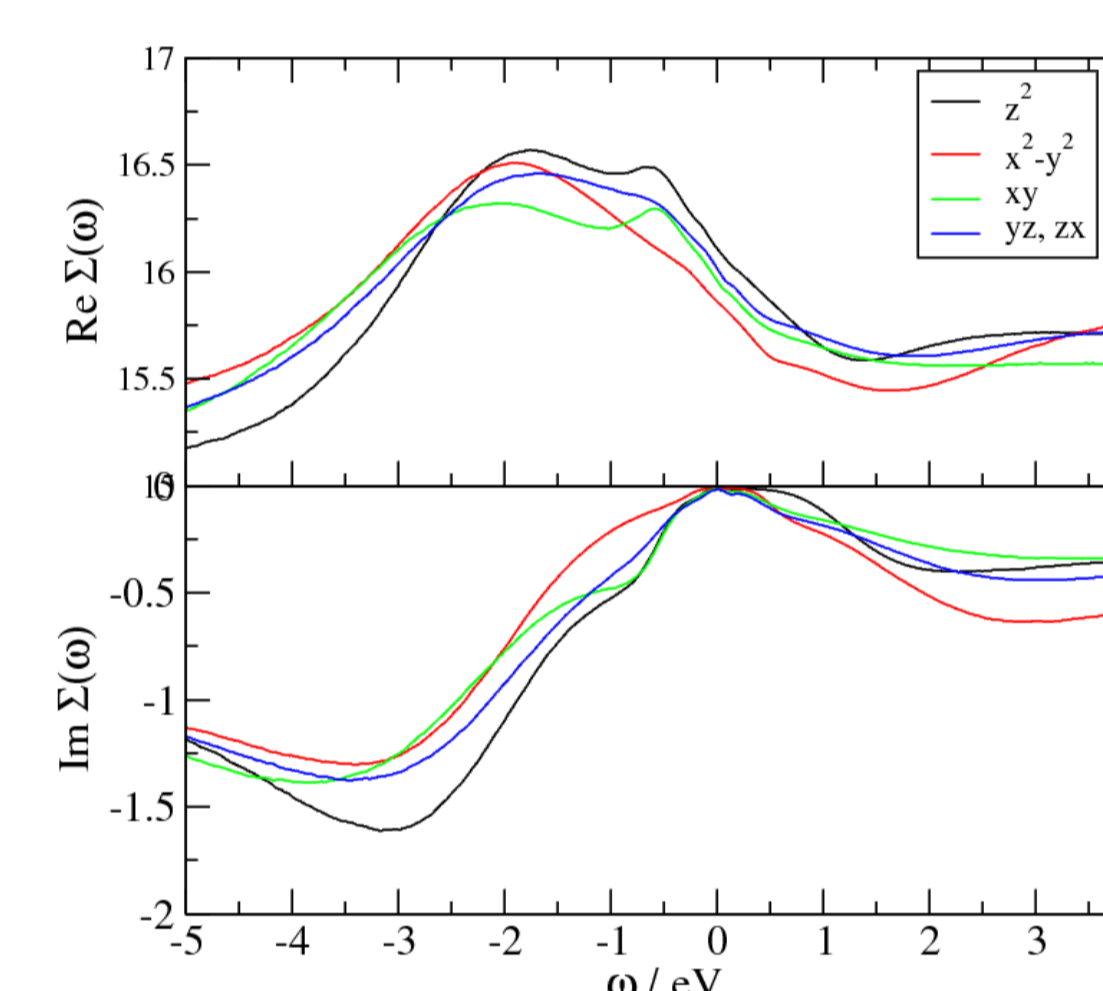
Projection operator matrix elements

$$P_{m\nu}^{\alpha,\sigma} = \langle w_{km}^{\alpha,\sigma} | \psi_{k\nu}^{\sigma} \rangle$$

Projected Green function

$$G_{mm'}^{\sigma, loc}(i\omega_n) = \sum_{k, \nu, \nu'} P_{m\nu}^{\alpha,\sigma}(\mathbf{k}) G_{\nu\nu'}^{\sigma}(\mathbf{k}, i\omega_n) P_{\nu'm'}^{\alpha,\sigma*}(\mathbf{k})$$

Self-Energy, Spectral function



Analytic continuation of the self energy:

$$\Sigma(i\omega) \rightarrow \Sigma(\omega + i\delta)$$

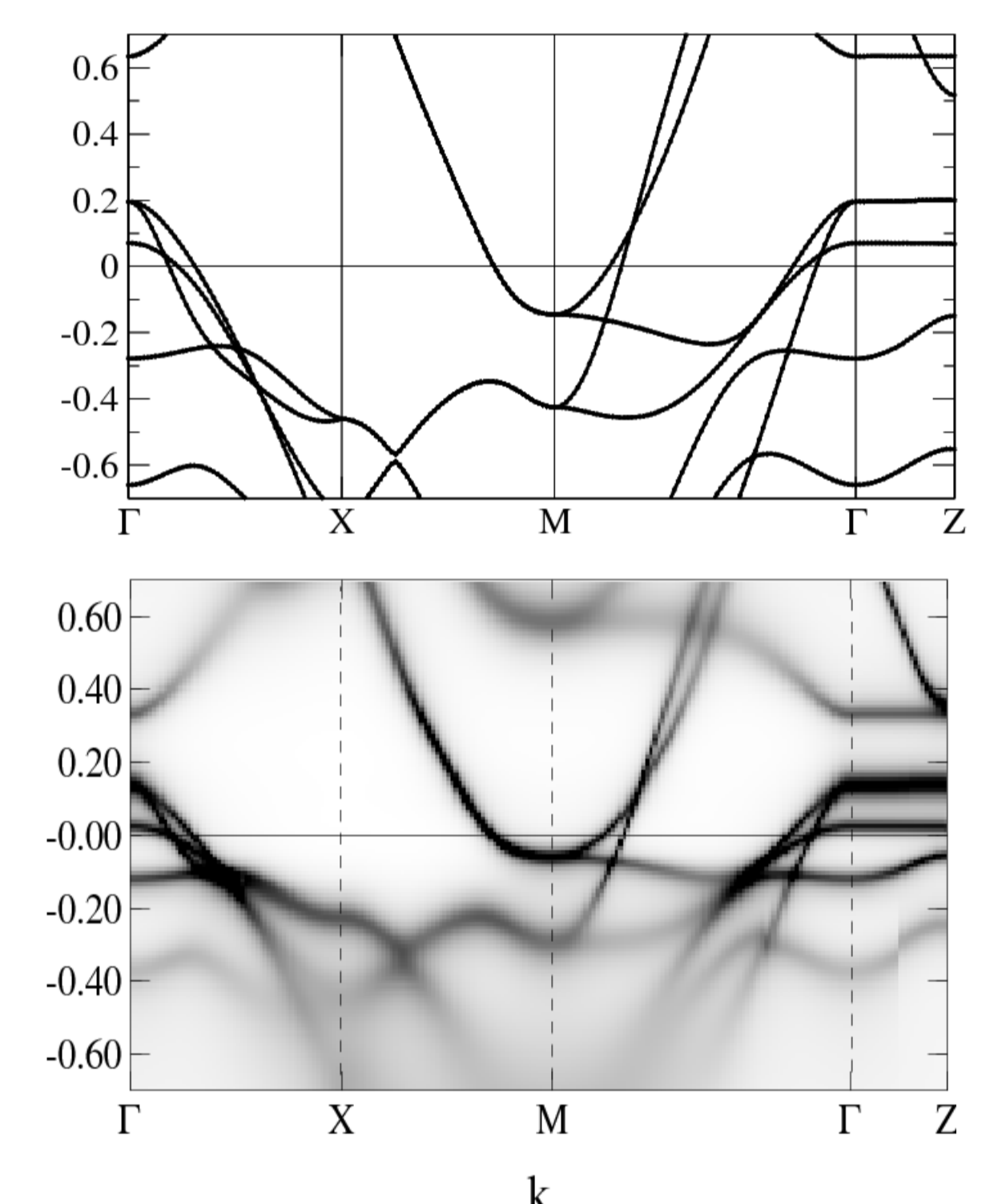
By stochastic Maximum Entropy
(K.S.D. Beach, arXiv:cond-mat/0403055)

Around $\omega = 0$:

Linear behavior of real part

Small imaginary part,
dispersing quadratically

→ Indication of Fermi liquid behavior



well-defined quasi-particles around Fermi level

Spread-out excitation for $\omega < -0.4$ eV due to
increased scattering rate (Im Σ)

Crystal field splitting: d_{z^2} and $d_{x^2-y^2}$ shift (cf LDA)

LDA+DMFT concept and the Impurity Problem

DFT part (Wien2K):
Solve Kohn-Sham Equations
 $\Rightarrow H_{\nu}(\mathbf{k}), |\psi_{k\nu}\rangle$

Interfacing:
Construct local orbitals
and projectors $P_{m\nu}^{\alpha,\sigma}(\mathbf{k})$

No re-interfacing with
electronic structure calculation

No full self-consistency

One-shot LDA+DMFT

DFT method:
Wien2K: Full Potential Linearized
Augmented Plane Wave code

DMFT part:

Imp. Solver: $\mathcal{G}_{mm'}^0(i\omega) \Rightarrow \Sigma_{mm'}^{\text{imp}}(i\omega)$

$$\Sigma_{\nu\nu'}^{\alpha,\sigma}(\mathbf{k}, i\omega_n) = \sum_{\alpha, m, m'} P_{\nu m}^{\alpha,\sigma}(\mathbf{k}) (\Sigma_{mm'}^{\text{imp}}(i\omega_n) - \Sigma^{\text{dc}}) P_{m'\nu'}^{\alpha,\sigma}(\mathbf{k})$$

$$G_{\nu\nu'}^{-1}(\mathbf{k}, i\omega_n) = (i\omega_n + \mu - \epsilon_{k\nu}) \delta_{\nu\nu'} - \Sigma_{\nu\nu'}^{\alpha,\sigma}(\mathbf{k}, i\omega_n)$$

$$G_{mm'}^{\text{loc}}(i\omega_n) = \sum_{k, \nu, \nu'} P_{m\nu}^{\alpha,\sigma}(\mathbf{k}) G_{\nu\nu'}^{\sigma}(\mathbf{k}, i\omega_n) P_{\nu'm'}^{\alpha,\sigma*}(\mathbf{k})$$

New Bath Greens function: $\mathcal{G}_0^{-1} = \Sigma_{\text{imp}} + G_{\text{loc}}^{-1}$

SC condition: $G_{mm'}^{\text{loc}} = G_{mm'}^{\text{imp}}$

Interaction Hamiltonian (density-density): $H_{\text{int}} = \frac{1}{2} \sum_{mm', \sigma\sigma'} U_{m,m'}^{\sigma\sigma'} n_{m\sigma} n_{m'\sigma'}$

$$U_{mm'}^{\sigma\bar{\sigma}} = U_{mm'mm'}, \quad U_{mm'}^{\sigma\sigma} = U_{mm'mm'} - U_{mm'm'm}$$

4-index U -matrix constructed from Slater integrals: $F^0 = U, \quad J = (F^2 + F^4)/14, \quad F^4/F^2 = 0.625$

Impurity Solver: **Continuous Time Quantum Monte Carlo**

Hybridisation expansion (P. Werner et al., 2006): Very efficient solver for quantum impurity problems

Density-Density interactions:
Maximum number of conserved quantities
Efficient update scheme ("Segment picture")

Inverse temperature reachable:
 $\beta = 40 \text{ eV}^{-1}$ without problems

Dependence on Wannier functions and Hund coupling

dpp-Hamiltonian:

$U = 2.69$ eV, $J = 0.79$ eV: $\langle Z \rangle = 0.62$

$U = 3.69$ eV, $J = 0.58$ eV: $\langle Z \rangle = 0.67$

$U = 3.69$ eV, $J = 0.80$ eV: $\langle Z \rangle = 0.53$

$U = 5.00$ eV, $J = 0.80$ eV: $\langle Z \rangle = 0.42$

Huge Hamiltonian (60 bands):

(U and J expected to be slightly larger):

$U = 3.69$ eV, $J = 0.80$ eV: $\langle Z \rangle = 0.56$

$U = 3.00$ eV, $J = 0.80$ eV: $\langle Z \rangle = 0.60$

$U = 3.00$ eV, $J = 0.60$ eV: $\langle Z \rangle = 0.73$

→ Not close to a Mott transition, converged in terms of Wannier function construction

d-Hamiltonian (10 Fe-d bands only):

$U = 4.00$ eV, $J = 0.70$ eV: $\langle Z \rangle = 0.11 - 0.35$

consistent with Haule et al.

$U = 2.42$ eV, $J = 0.43$ eV: $\langle Z \rangle = 0.5 - 0.6$

Strong dependence on J (artefact?)

Problems with *d*-only Hamiltonian:
Delocalized Wannier orbitals!
Anisotropic interaction matrices!
How good is LDA+DMFT here?

Rotational invariant Hund coupling:

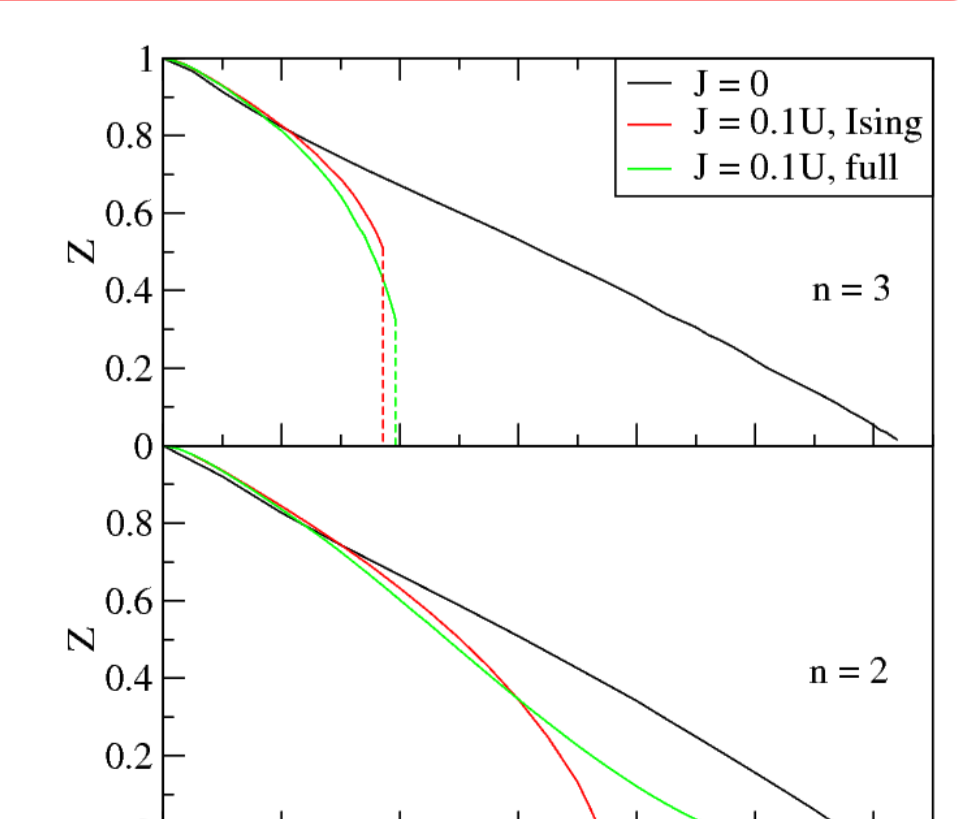
Neglected terms:

$$H_{\text{sf+ph}} = -\frac{J}{2} \sum_{mm'} (c_{m\uparrow}^\dagger c_{m'\downarrow}^\dagger c_{m'\uparrow} c_{m\downarrow} + c_{m\downarrow}^\dagger c_{m'\uparrow}^\dagger c_{m'\downarrow} c_{m\uparrow} + \text{h.c.})$$

Negligible influence for
moderate correlations, $Z = 0.5$

Important near
phase transition, $Z = 0.1-0.2$!

→ **No change in physical picture of
the Pnictide superconductors**



multiband Hubbard model for semicircular DOS
(self-energy functional theory)