Optical conductivity of Fe-pnictides in the SDW state.

What do we learn from DFT calculations?

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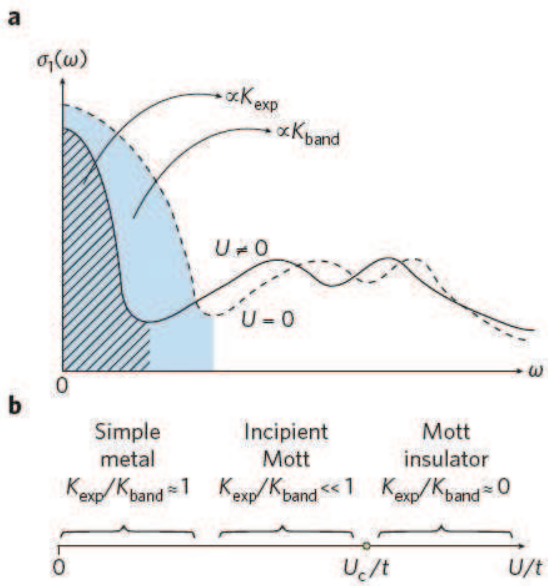
Financial support: **DFG**

PRB 82, 165102 (2010) **PRB(RC) 81, 220506 (2010)**

Optical conductivity

Electronic structure reflected by optical properties

- **Low frequency region:** **governed by itinerant carrier contribution,**
  $\rightarrow$ effect of correlations.
- **Infrared regime:** **dominated by gap features (SDW gap/ SC gap).**
- **Visible part of the spectrum:** **band structure in the normal state.**



Q. Si Nat. Phys. (2009), Degiorgi arXiv:1006.4698

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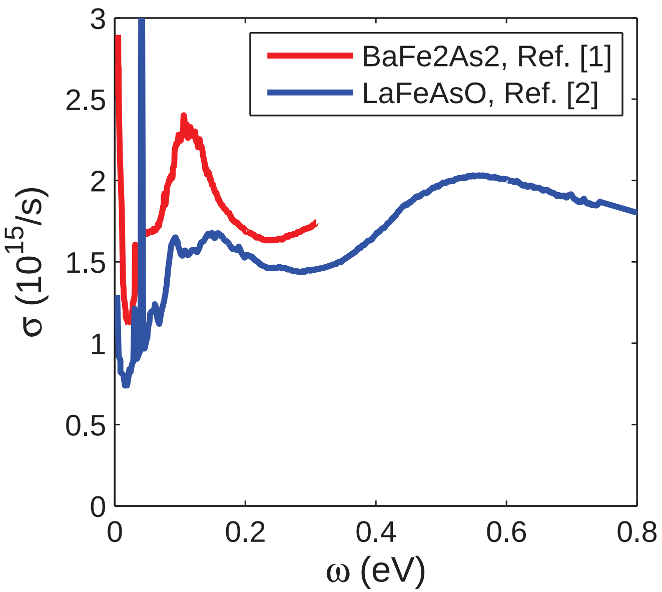
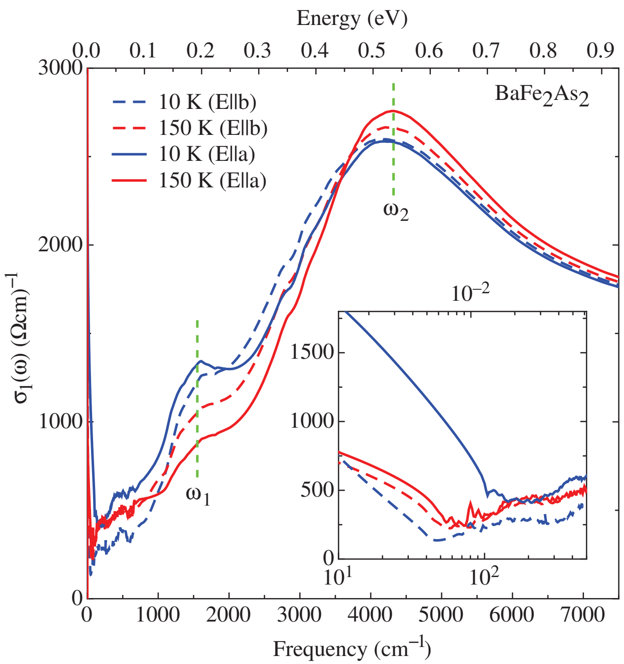


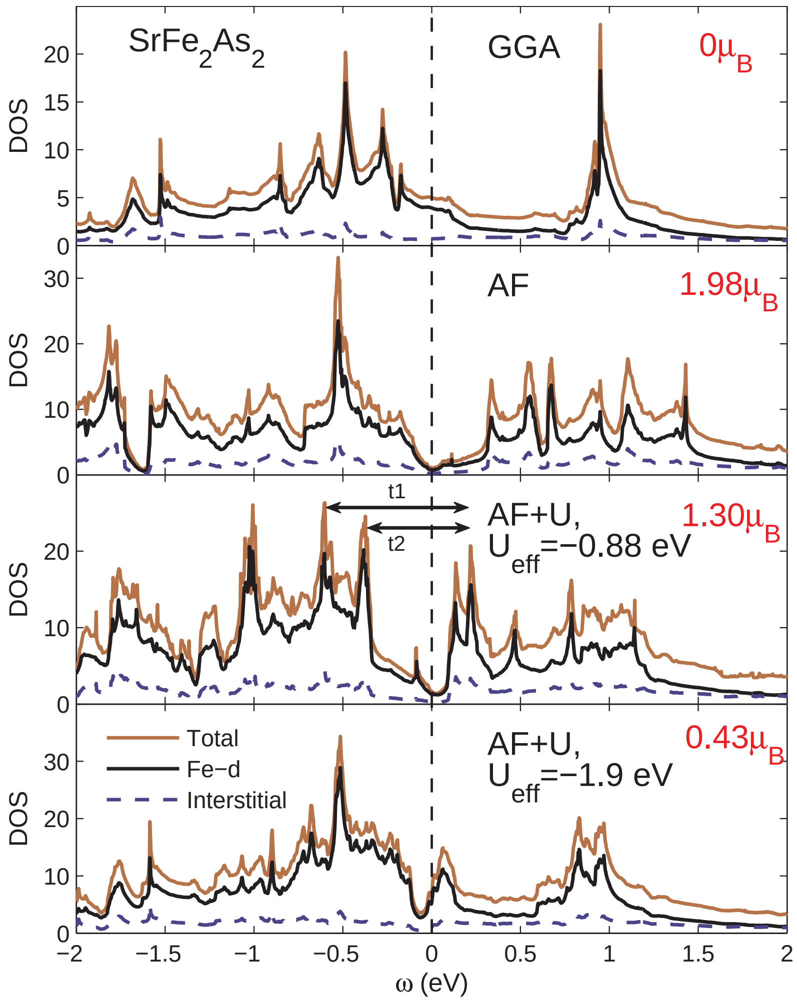


- **Metallic**
- **Peak at SDW gap frequency**
- **Broad peak in the midinfrared (persists above T_{SDW})**
- **Anisotropic dc response**

1. Hu *et al.* PRL (2008)
2. Chen *et al.* PRB (2010)

Dusza *et al.* arXiv:1007.2543

DFT for Fe-pnictides: reduced magnetic moment



- **Wiener2k GGA+U_{eff}** $\quad U_{eff} = U - J$

  atomic limit double-counting correction:

  $$\frac{U-J}{2}\sum_\sigma n_{m\sigma}(1-n_{m\sigma})$$

  - $U_{eff} > 0$ **'reproduces' Mott gap in correlated insulators**
  - $U_{eff} < 0$ **'reduces' magnetic moment**
    - **reduces SDW gap size**
    - **increases dc conductivity**

exp. $\mu = 1.0\mu_B$

Jesche *et al.* PRB (2008).

Linear optical response

$$Im\varepsilon_{ii}^{\text{inter}}(\omega) = \frac{\hbar^2 e^2}{\pi m^2 \omega^2} \sum_{v,c} \int_{\vec{k}} |p_{i;c,v,\vec{k}}|^2 \delta(E_{c,\vec{k}} - E_{v,\vec{k}} - \hbar\omega). \qquad (1)$$

$$p_{i;n,n',\vec{k}} = \langle n, \vec{k} | p_i | n', \vec{k} \rangle$$

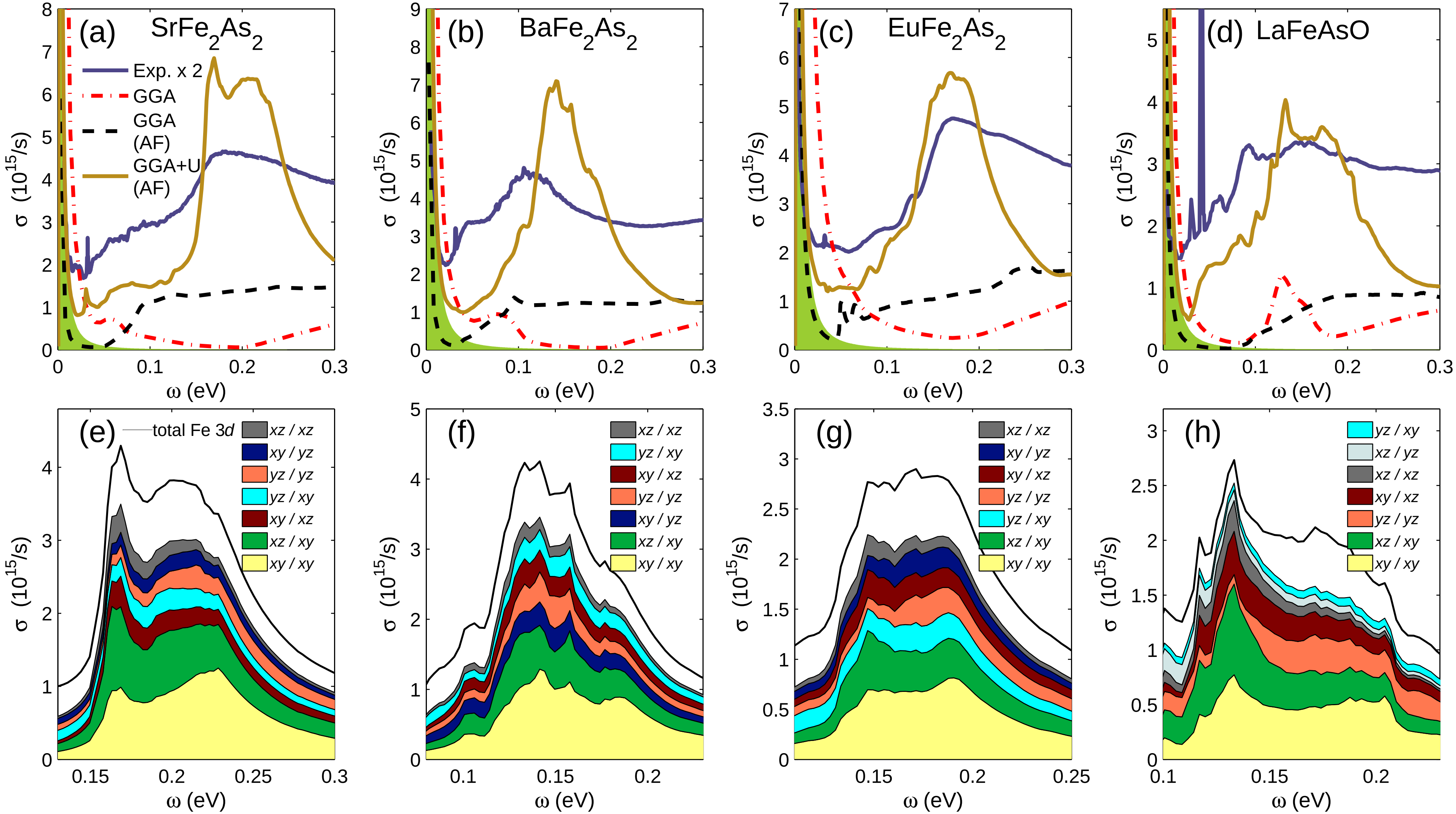
$$Re\sigma_{ij}(\omega) = \frac{\omega}{4\pi} Im\varepsilon_{ij}(\omega). \qquad (2)$$

Random Phase Approximation

- **KS orbitals**
- **dipole approximation**

Optical conductivity

DFT results Ferber *et al.* PRB (2010)

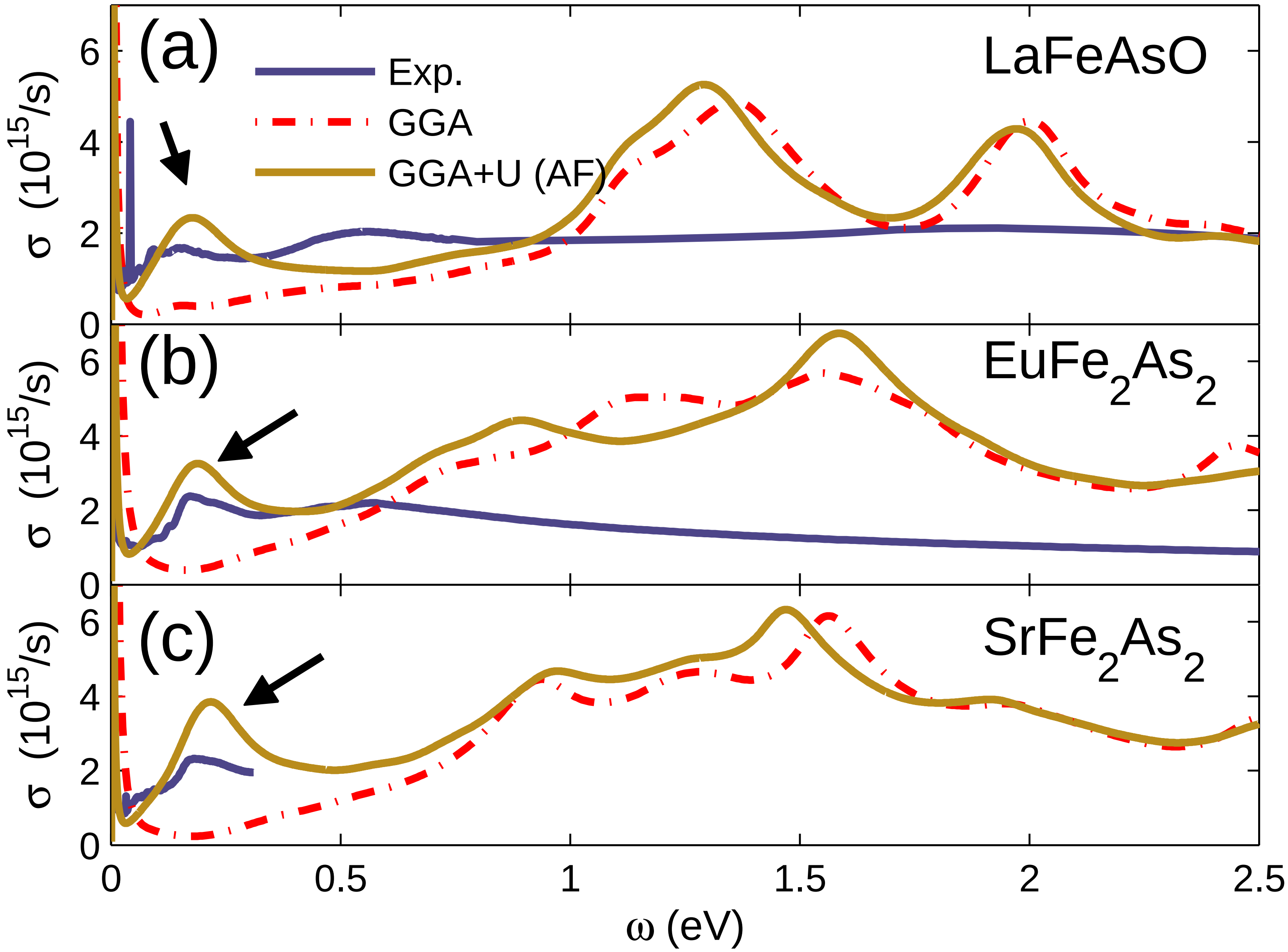


$SrFe_2As_2$ and $BaFe_2As_2$ Hu *et al.* PRL (2008) DFT Sanna *et al.* arXiv:1010.0220

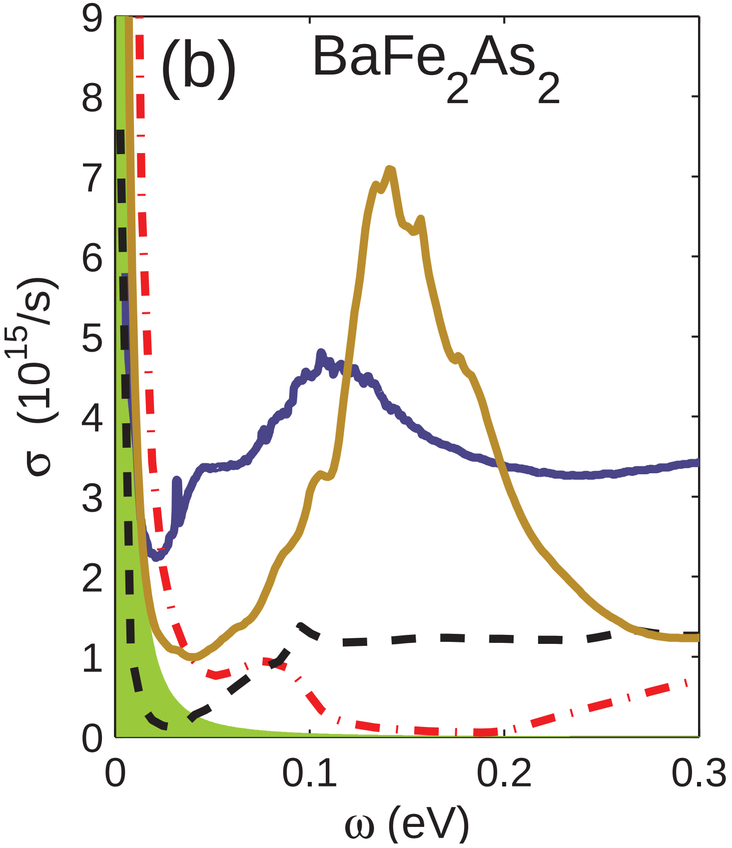
$EuFe_2As_2$ Wu *et al.* PRB (2010)

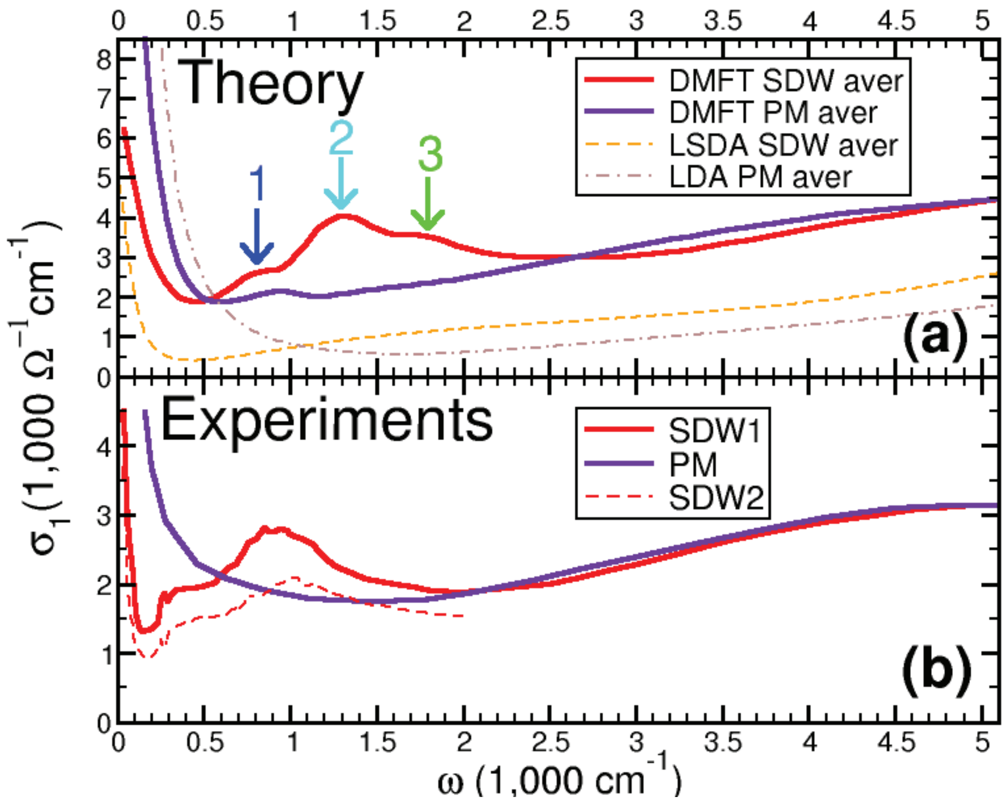
LaFeAsO Chen *et al.* PRB (2010).

Optical conductivity in the higher-energy region



$BaFe_2As_2$: Comparison DFT ↔ LDA+DMFT

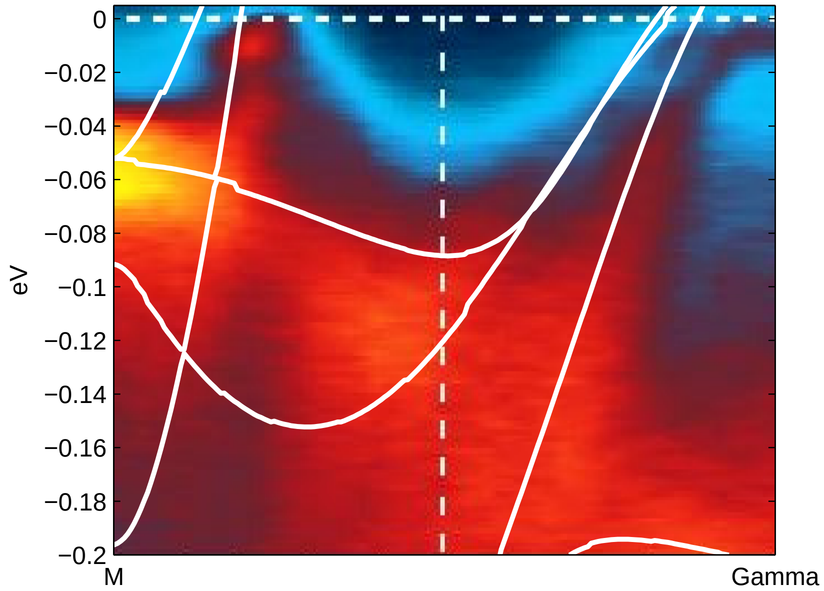




Yin, Haule, Kotliar arXiv:1007.2867

$BaFe_2As_2$: Comparison DFT $\leftrightarrow$ LDA+DMFT

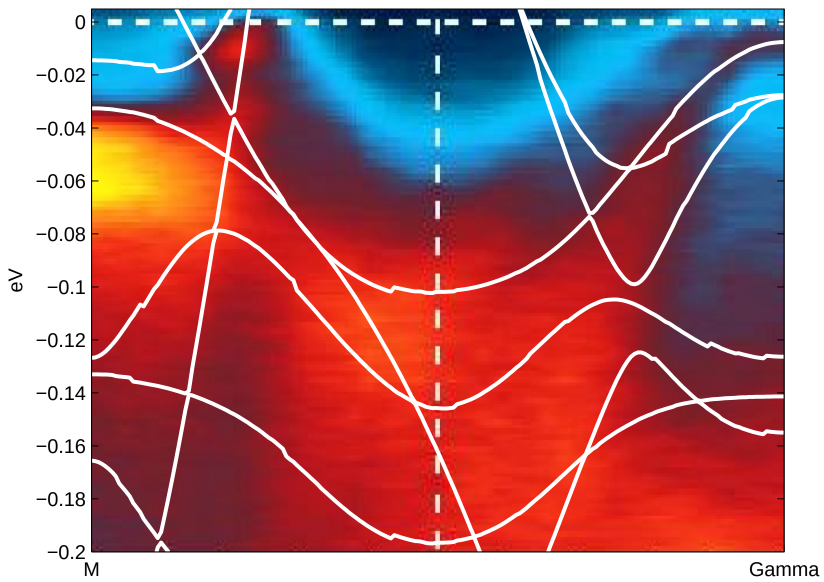
GGA

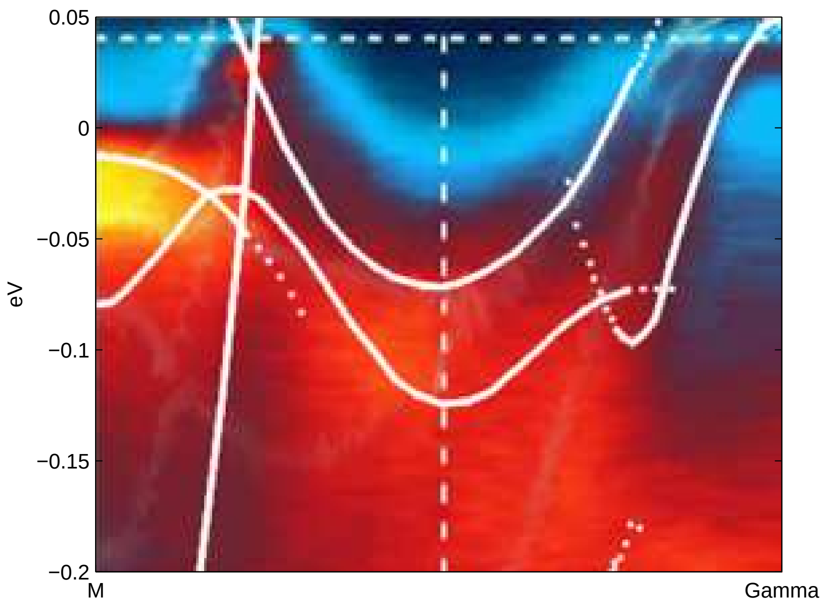


ARPES: Richard *et al.* PRL (2010)

LDA+DMFT Yin, Haule, Kotliar arXiv:1007.2867

GGA+ U_{eff}





Summary

- **DFT reproduces a number of features associated with the SDW state**
- **GGA + U_{eff} , $U_{eff} < 0$ reduces μ but doesn't distort the overall bandstructure**
- **agreement with low-frequency excitations**
- **Comparison DFT $\leftrightarrow$ LDA+DMFT**
  - **scaling in DFT results necessary**
- **Renormalization of kinetic energy:**
  - $K_{exp}/K_{band} = (\omega_p^{exp})^2/(\omega_p^{band})^2$
  - **f.i. $SrFe_2As_2$ $K_{exp}/K_{band} \sim$ 0.37 - 0.15 in the SDW state.**

$\rightarrow$ **significant correlations in the SDW state.**

- **Origin reduced magnetic moment? frustrated/unfrustrated bands? multiorbital?**

H. Lee *et al.* PRB (2010)