

Influence of interface mixing on magnetism of $\text{Au}_4\text{Co}_{11}$ multilayers

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- This study approaches the system from the other direction: Au as the starting point

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- Probing magnetism induced at the Au sites

Induced Au magnetism in $\text{Au}_4\text{Co}_{11}$

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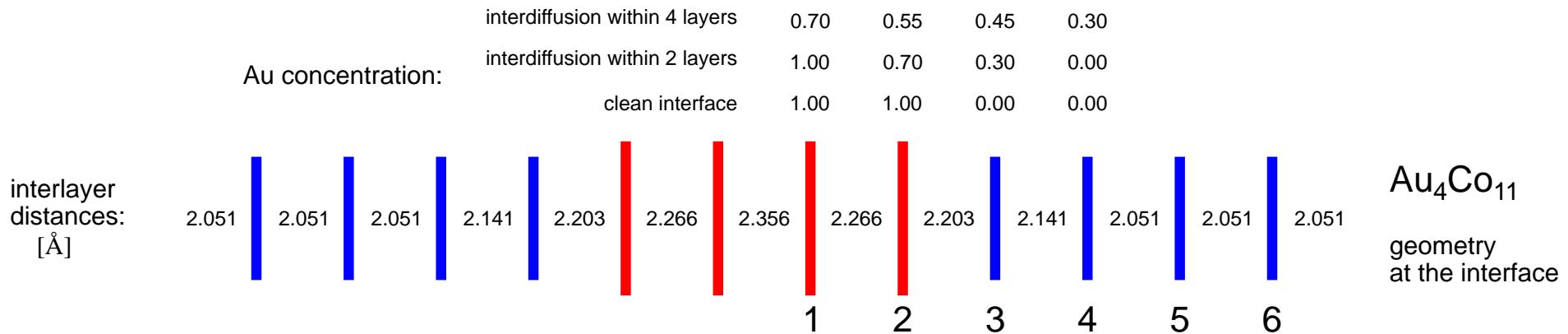
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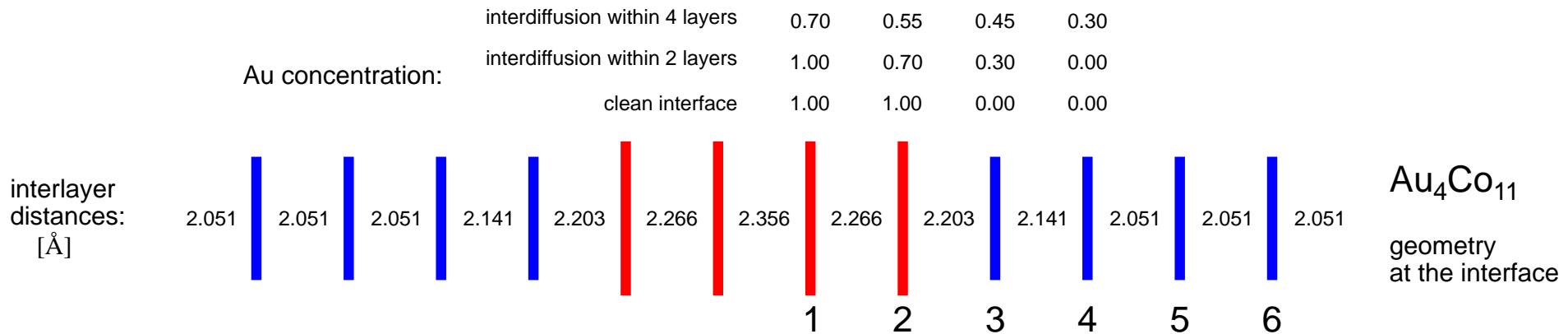
Geometry model

- fcc geometry, (111) interface, ABC stacking
- Intra-planar interatomic distances are identical for each layer (weighted average of Au and Co crystals)
- Distances between layers taken from experiment of F. Wilhelm *et al.*



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- For comparison, an auxiliary model $\text{Co}_4\text{Co}_{11}$ system is used (same geometry, all atoms are Co)

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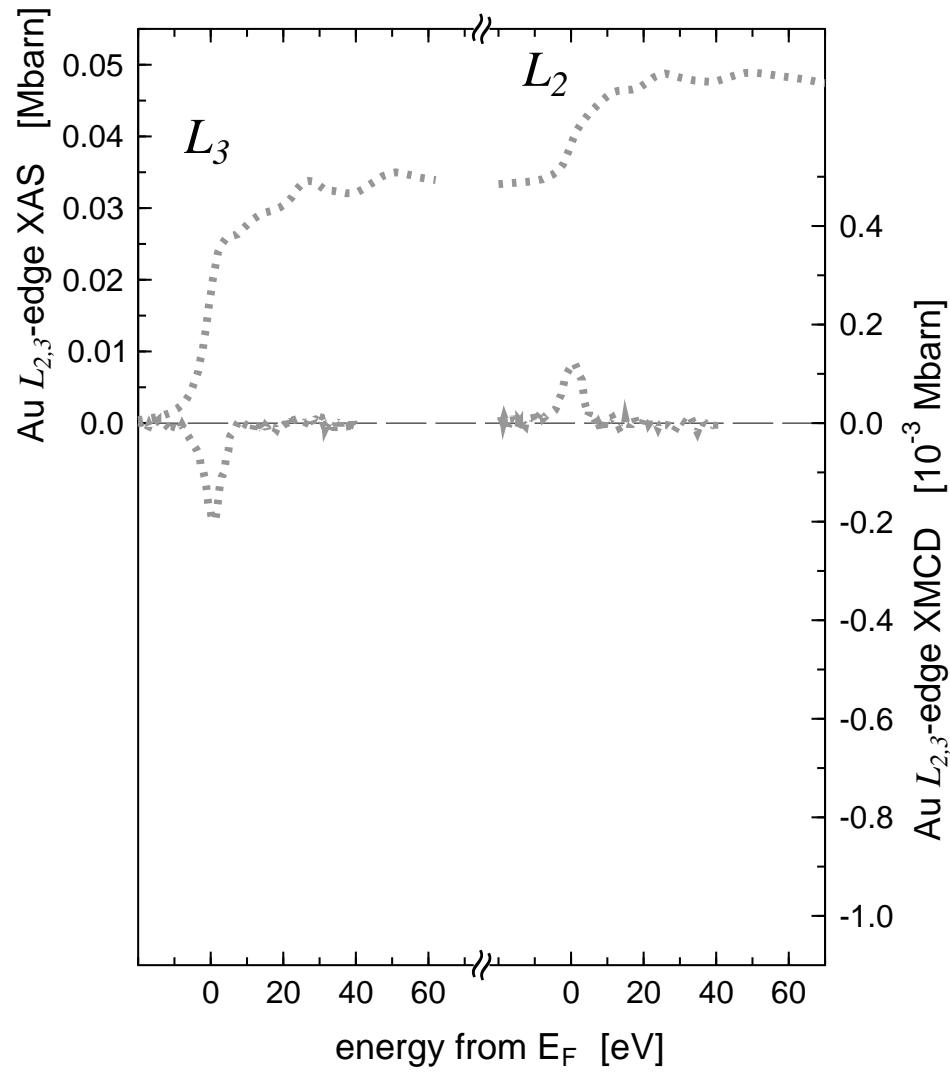
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<http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR>

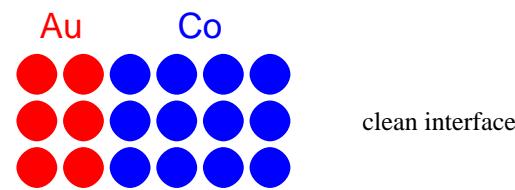
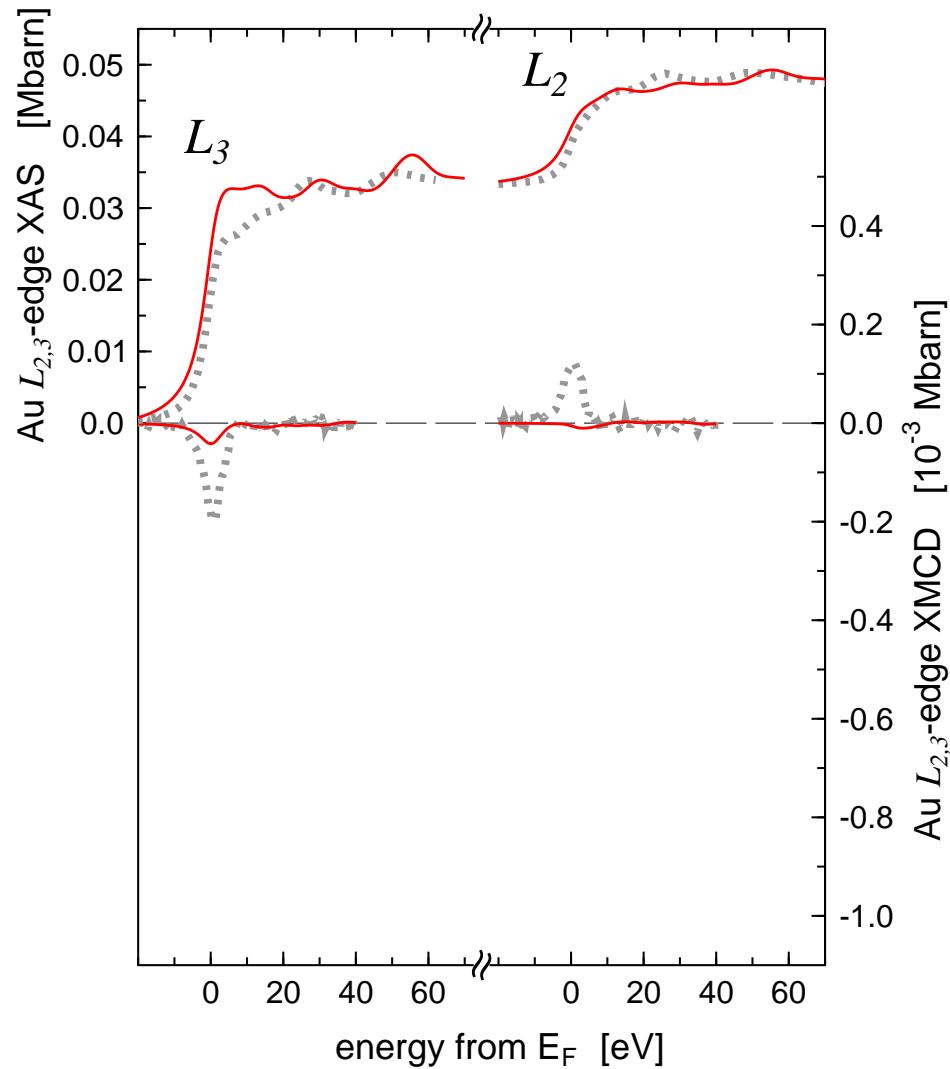
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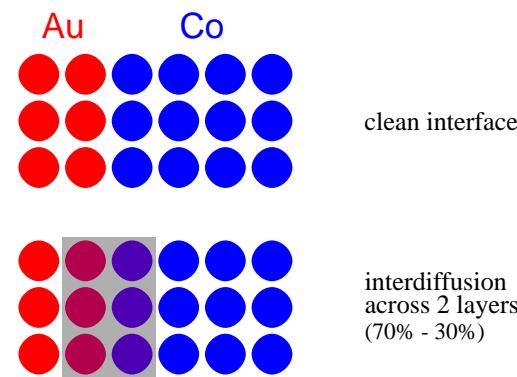
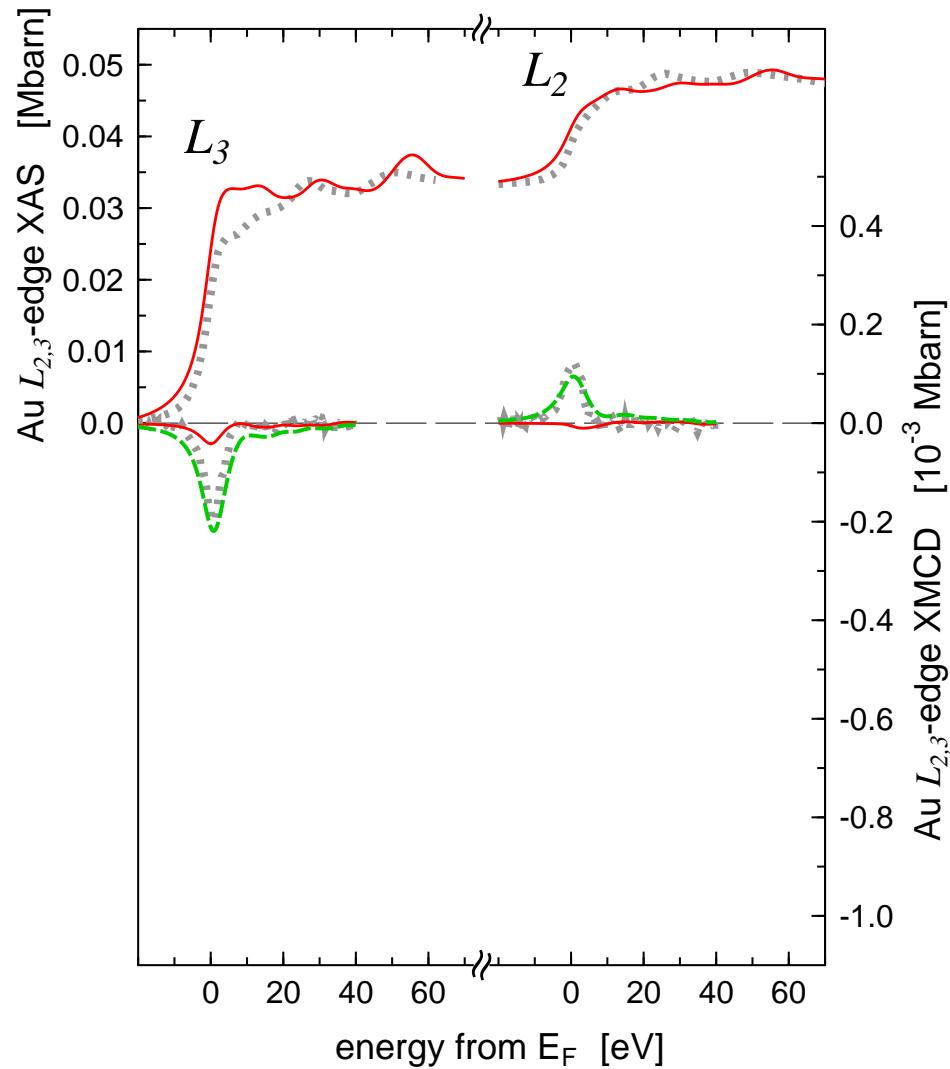
Au $L_{2,3}$ edge XAS and XMCD spectra



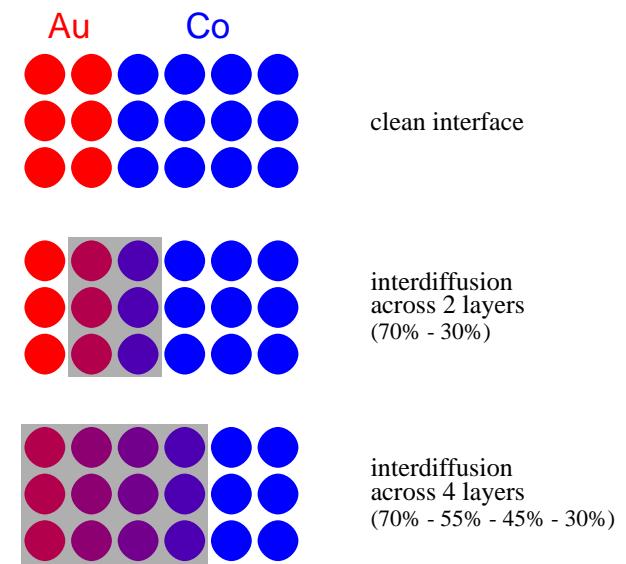
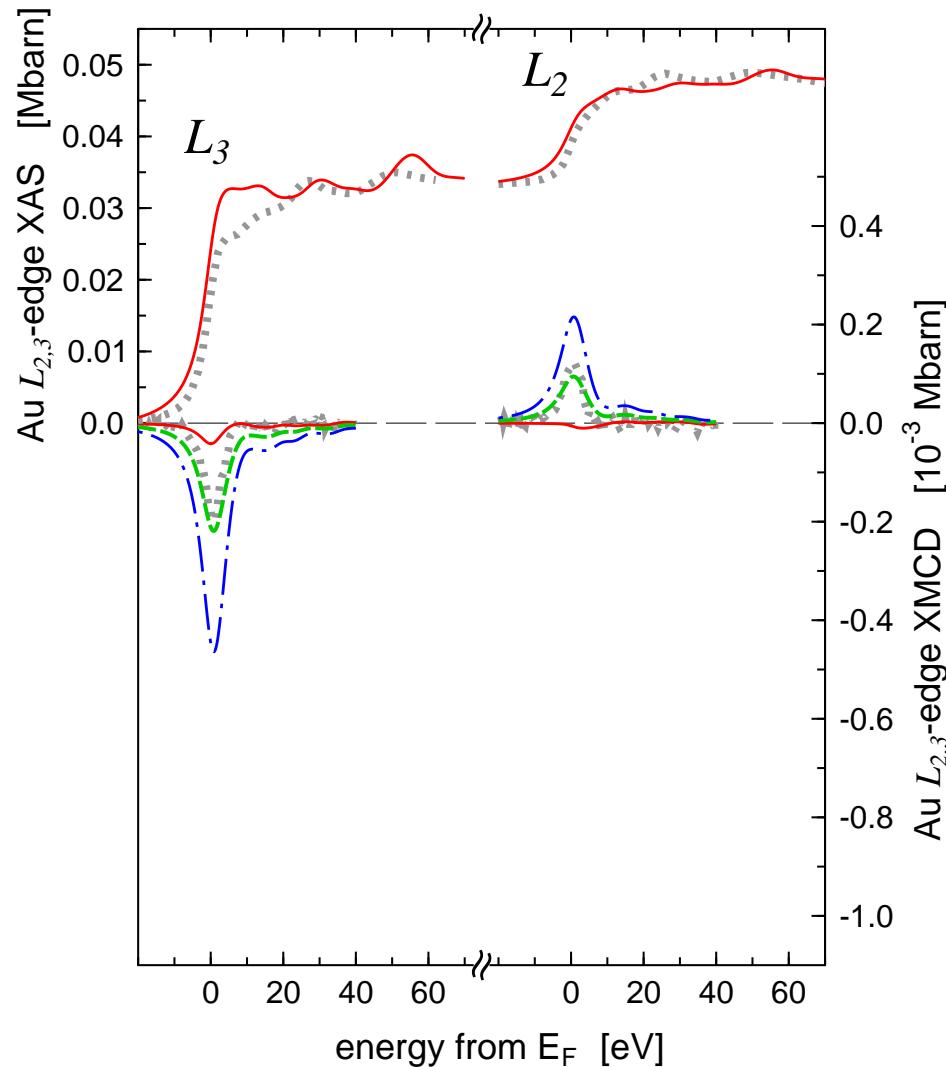
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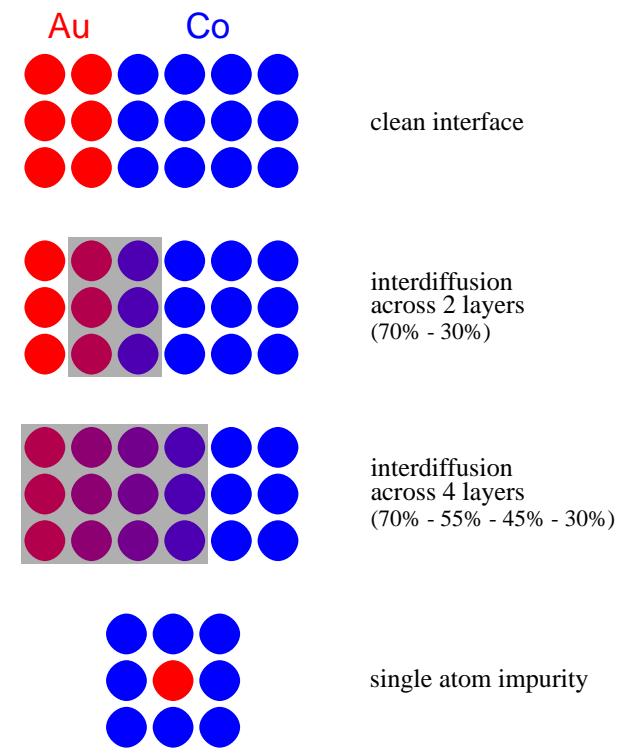
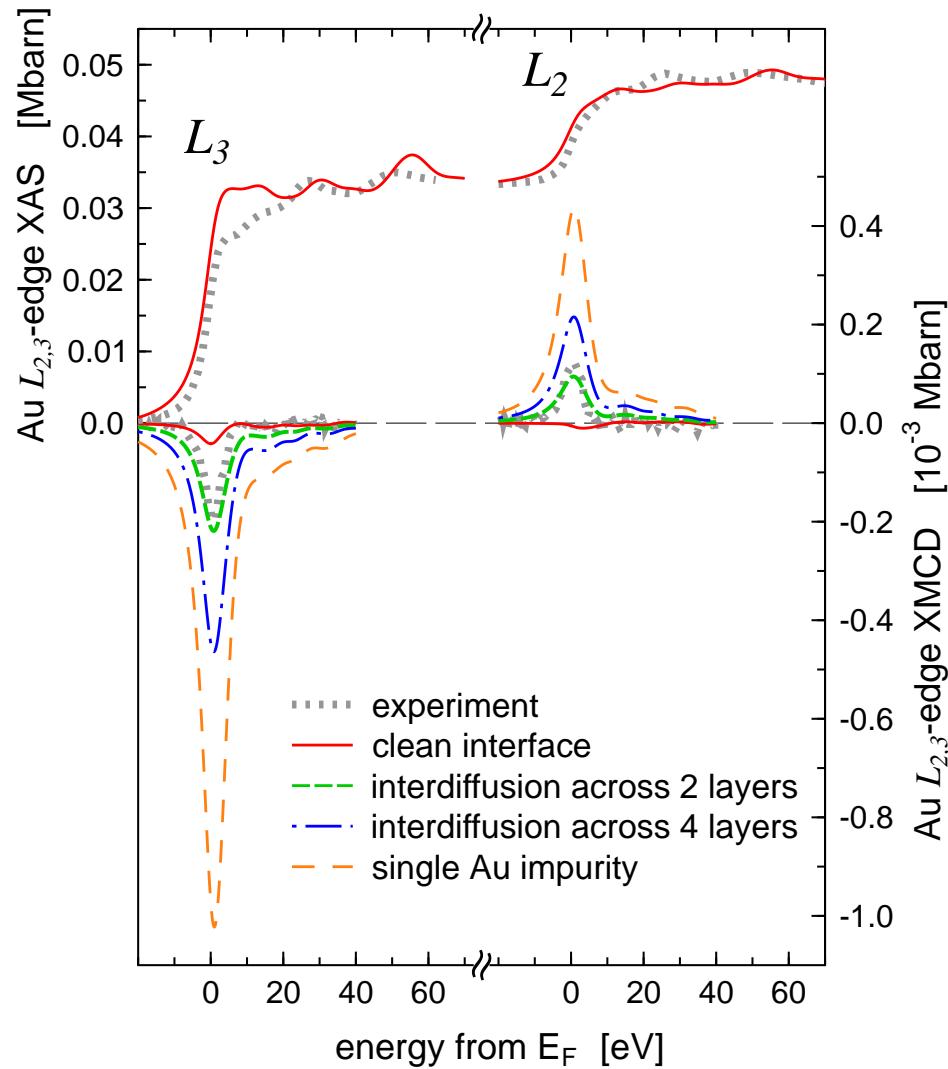
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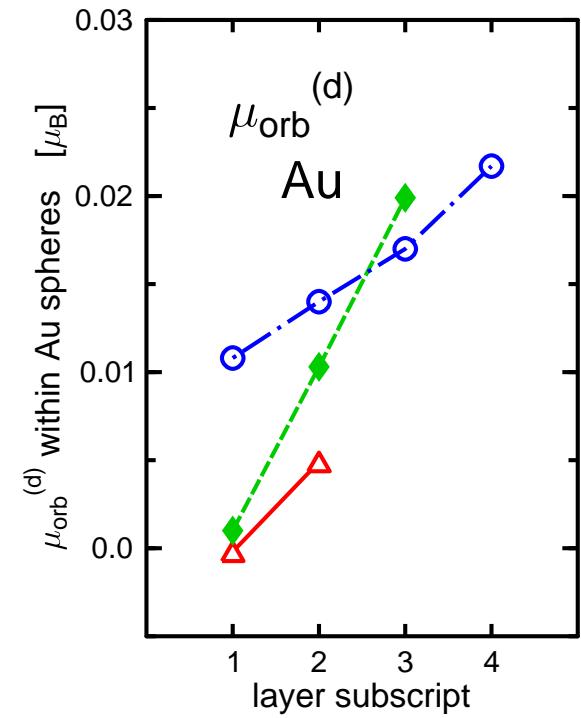
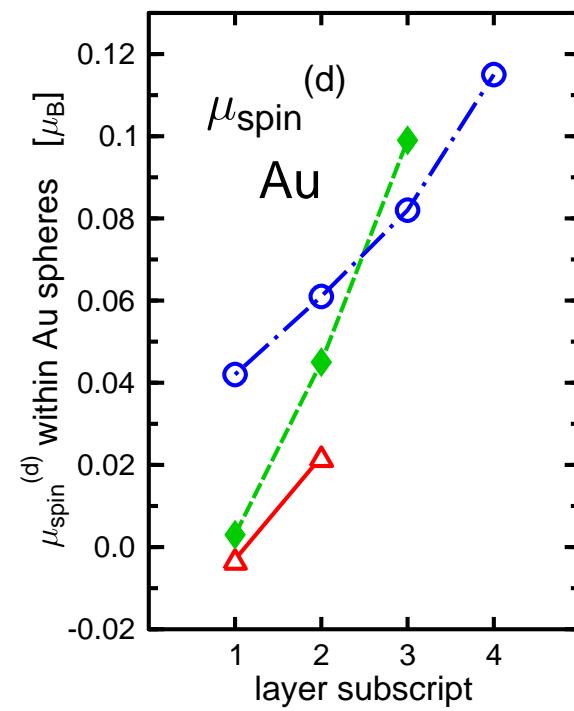
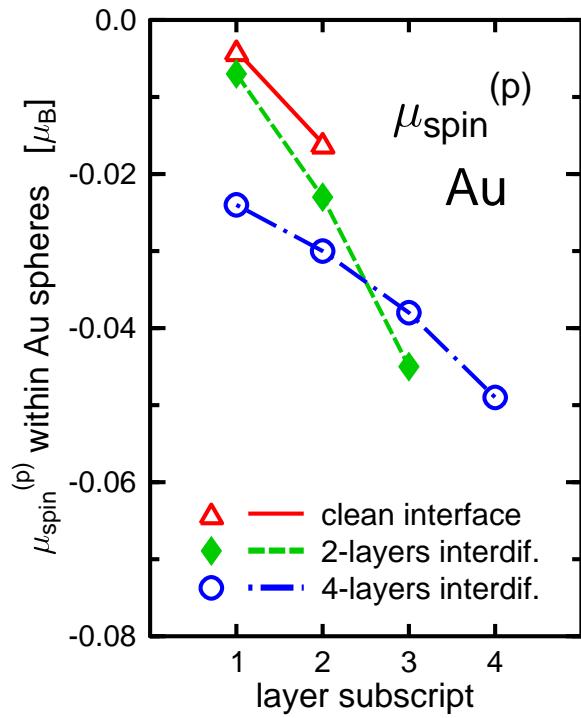


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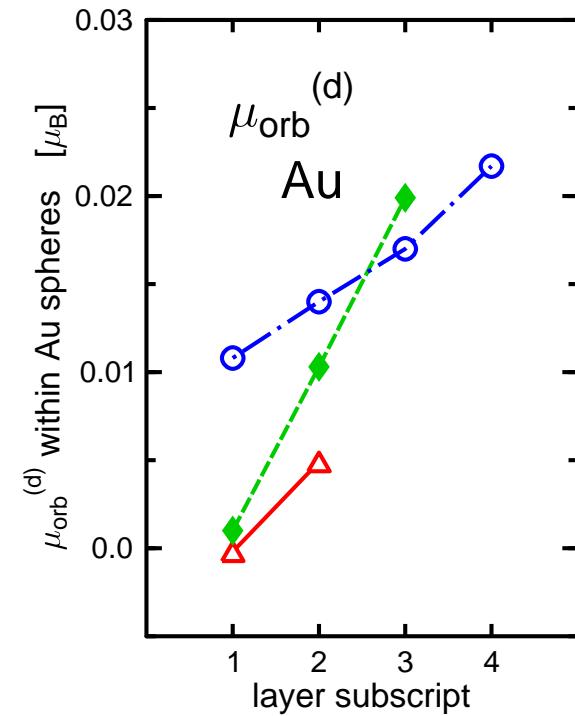
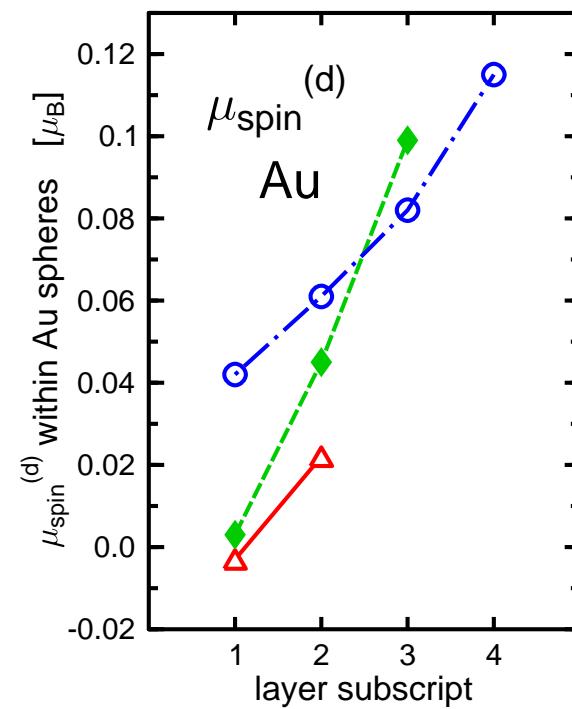
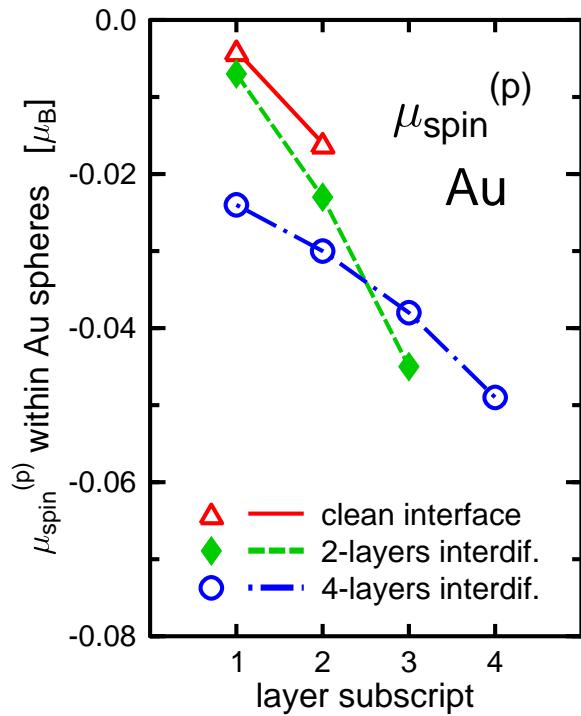
Local moments inside Au spheres

- p -component of μ_{spin} , d -component of μ_{spin} , d -component of μ_{orb}



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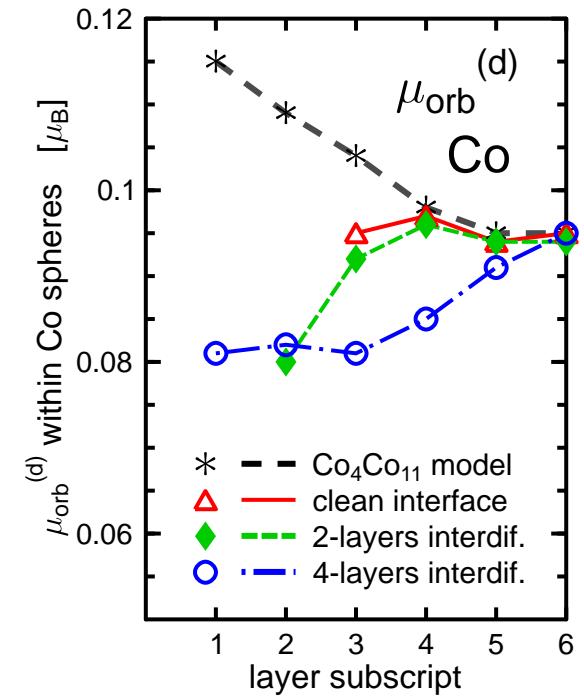
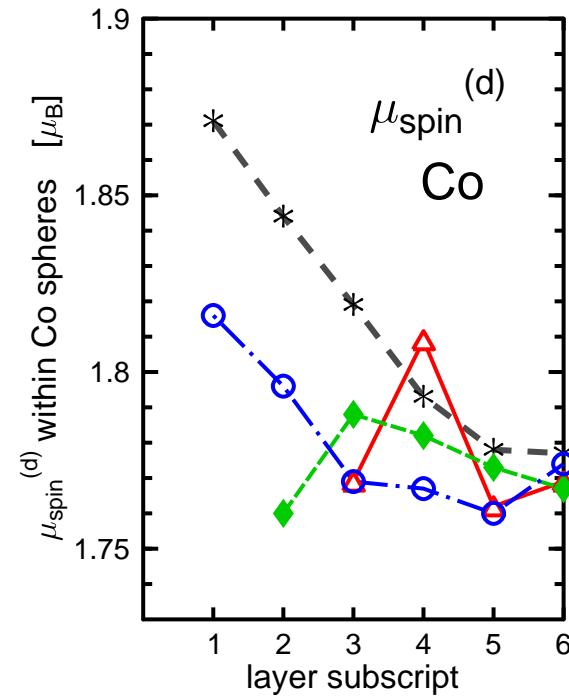
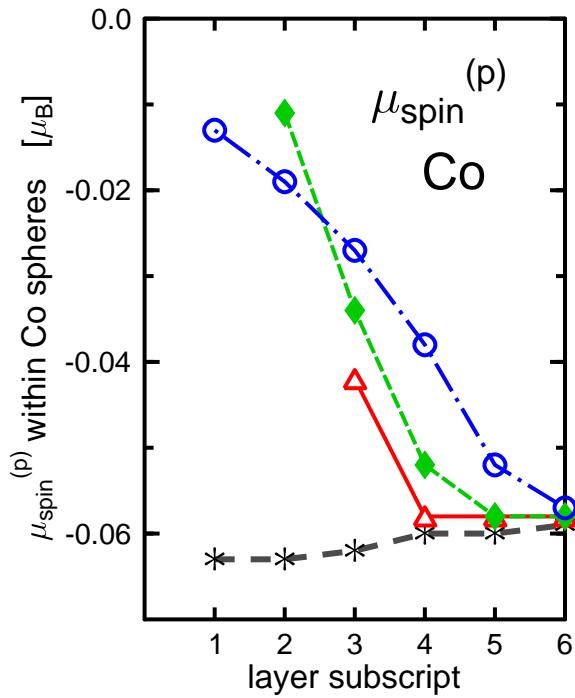
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- More Co means more magnetism

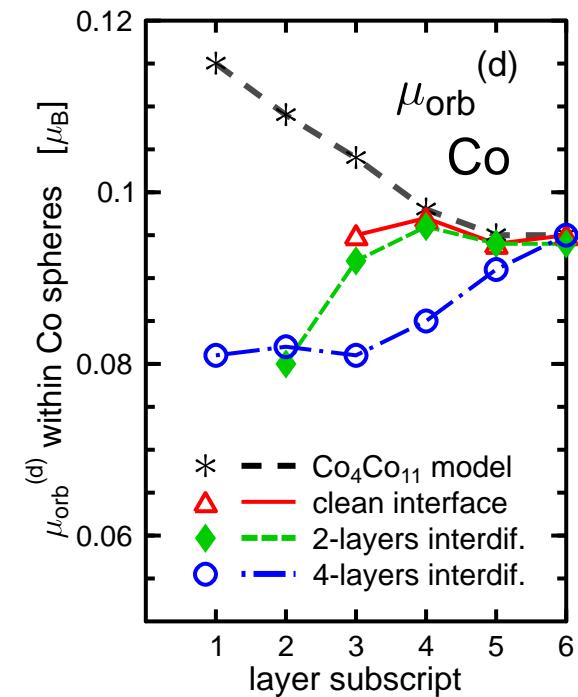
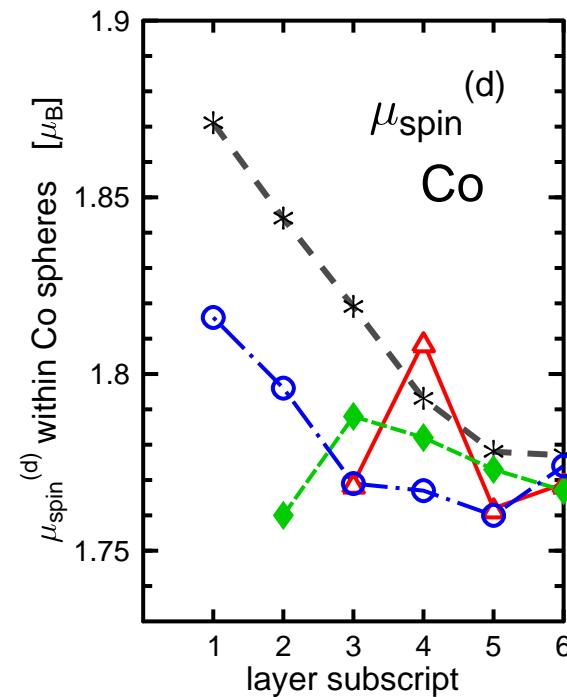
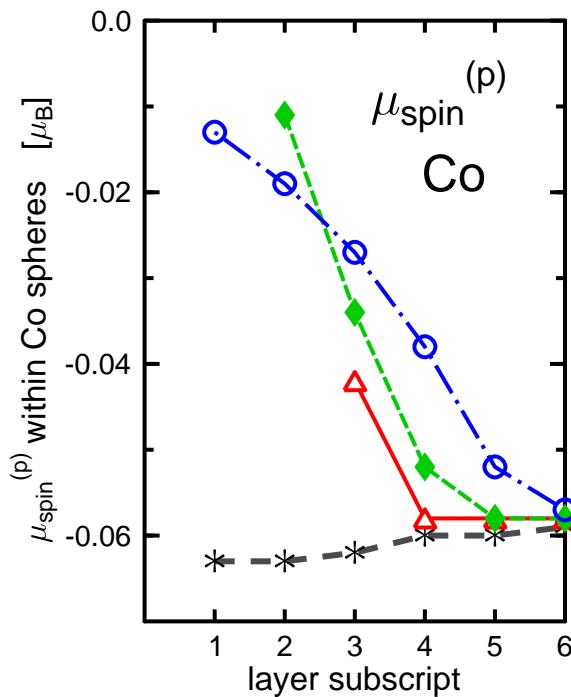
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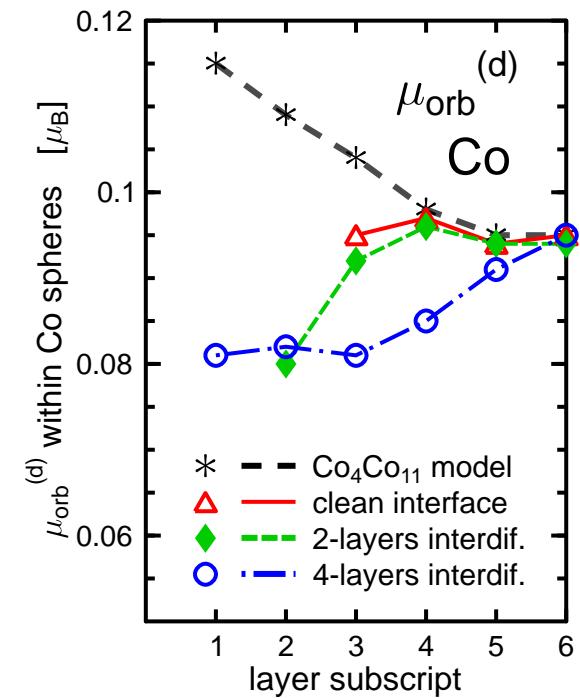
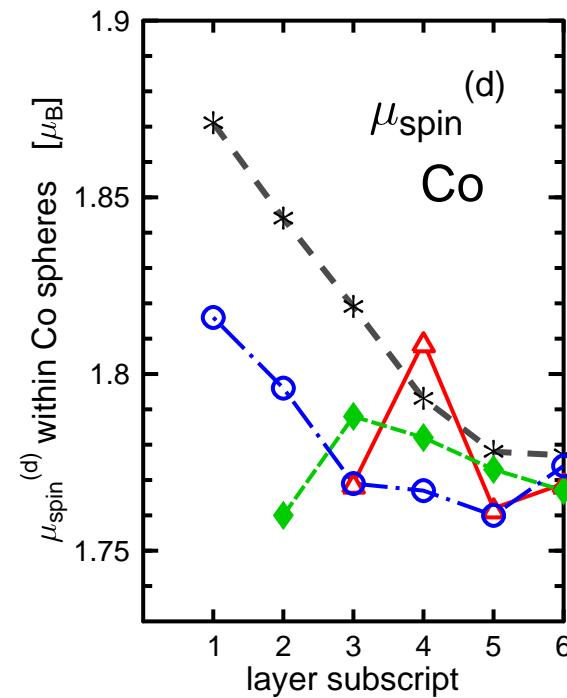
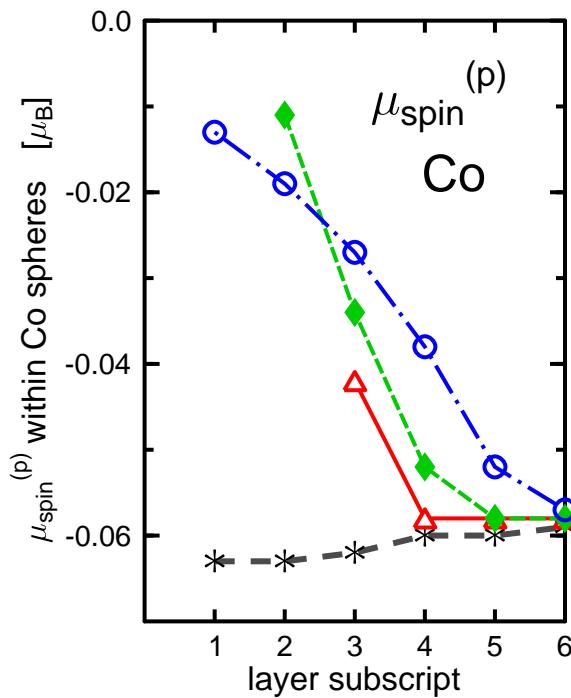
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- Lattice expansion enhances magnetism

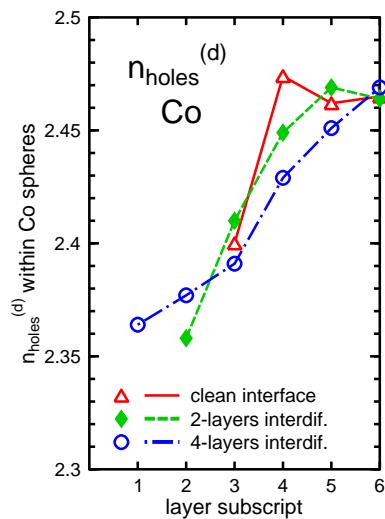
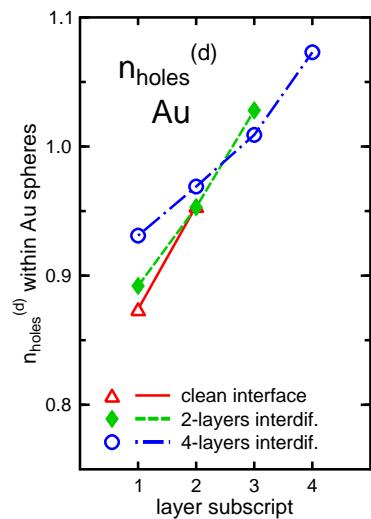
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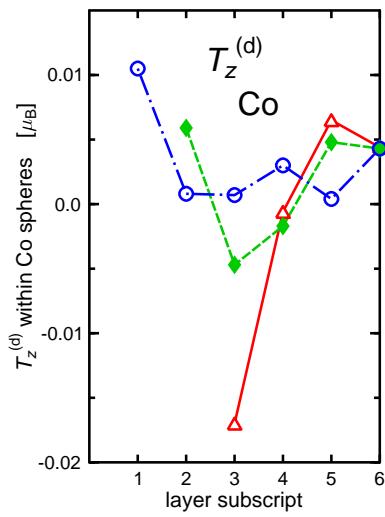
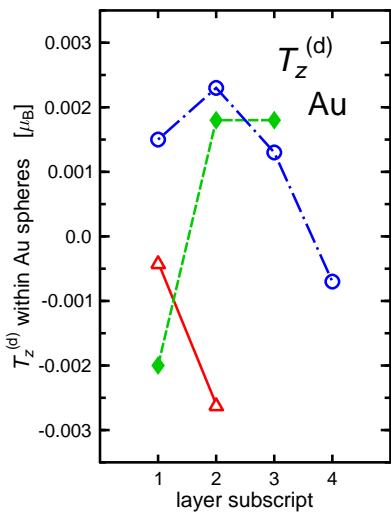


- Latice expansion enhances magnetism
- Chemistry complicates the geometry

Quantities related to sum rules

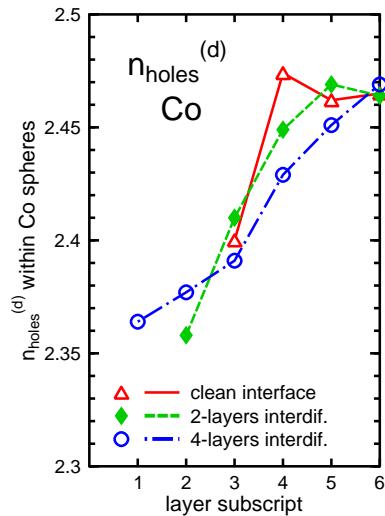
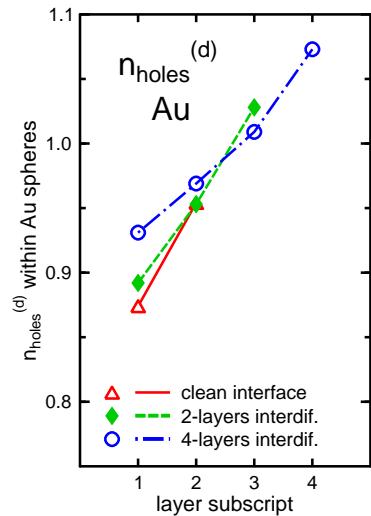


number of holes in the d -band

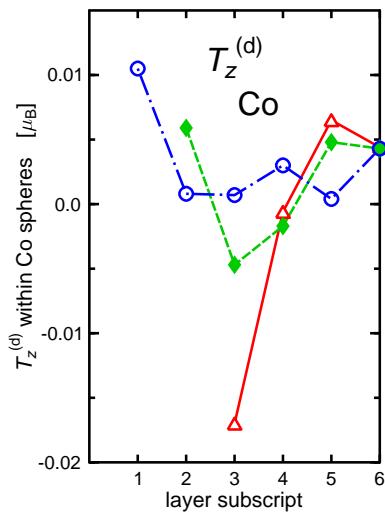
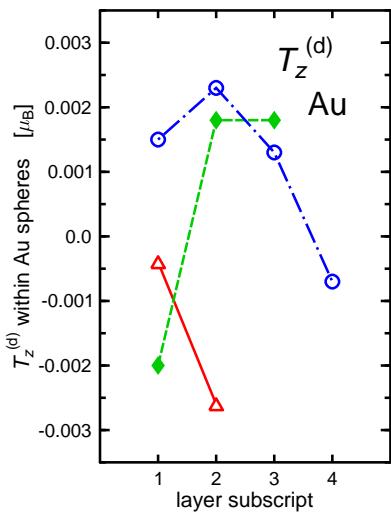


magnetic dipole term T_z
(d -component)

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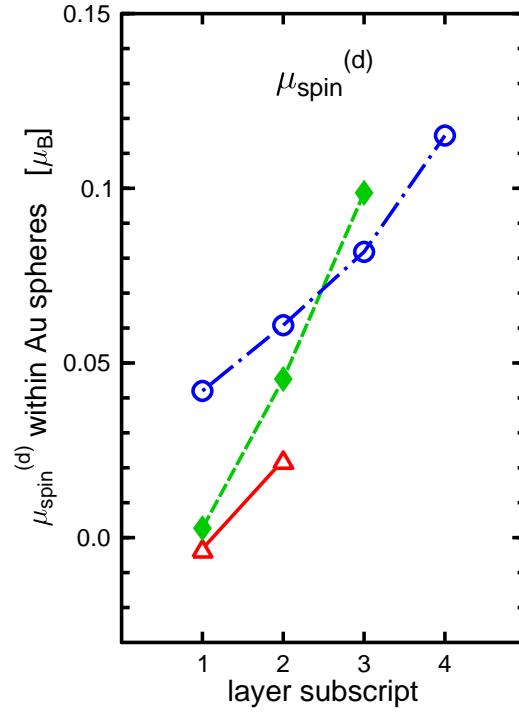
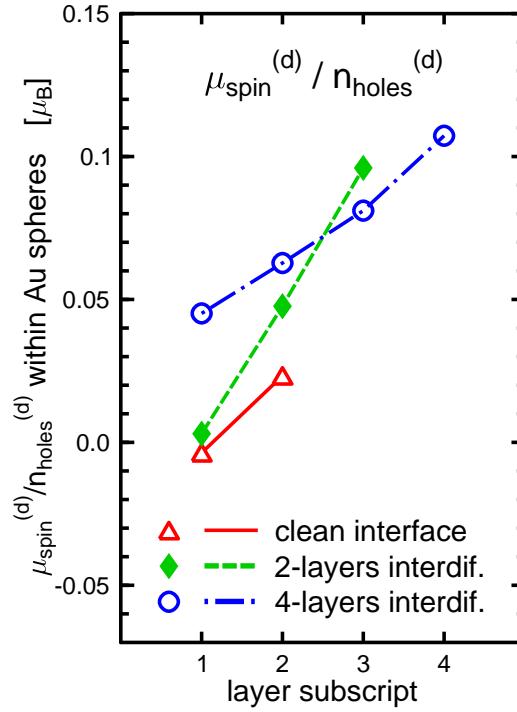
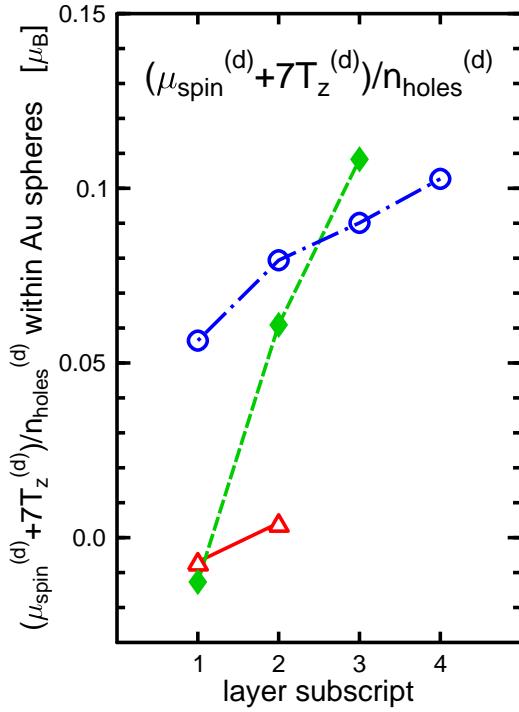
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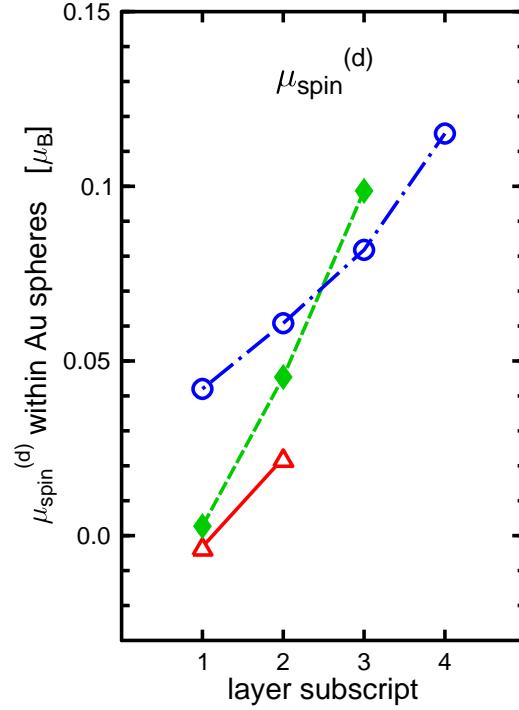
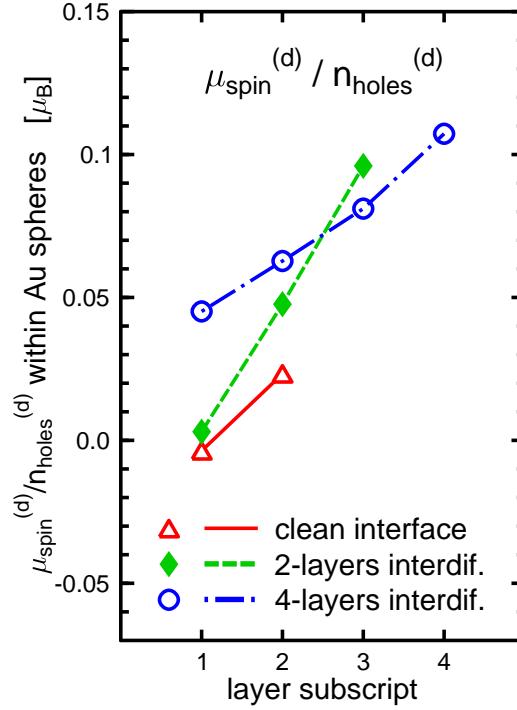
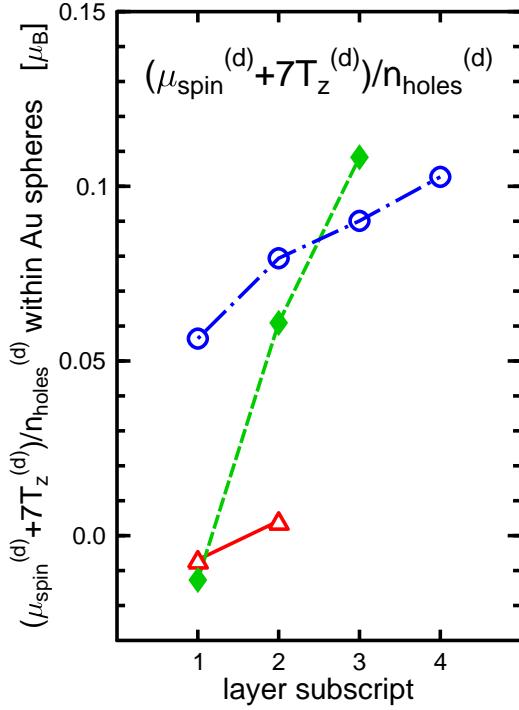
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- $n_{holes}^{(d)}$ and $T_z^{(d)}$ vary from site to site

Spin moment sum rule for Au sites

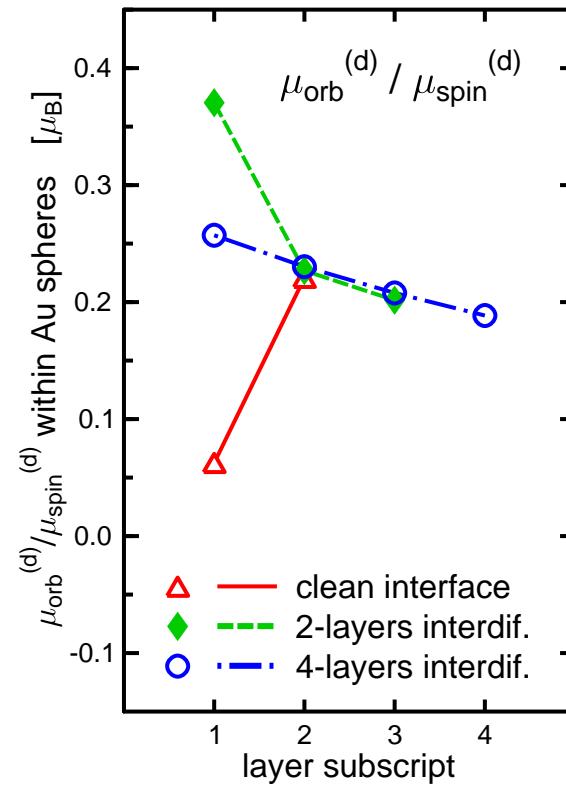
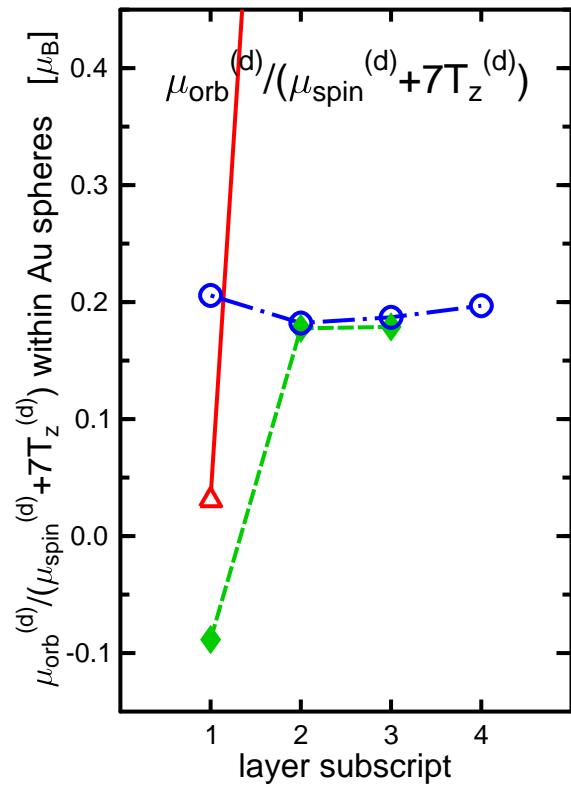


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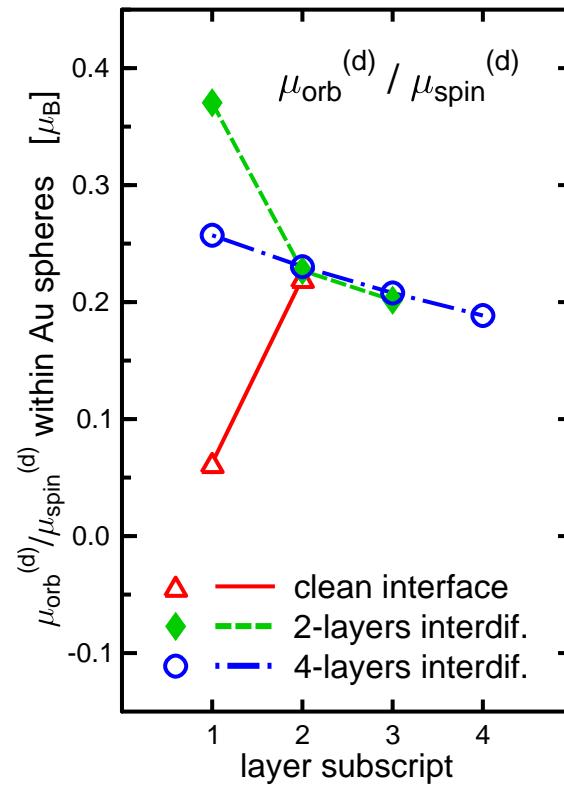
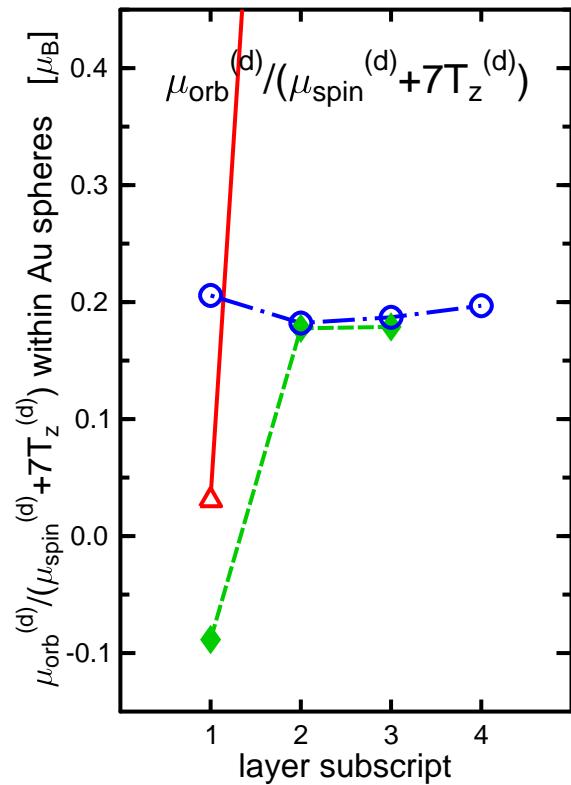


- Variations of $n_{\text{holes}}^{(d)}$ and $T_z^{(d)}$ do not really matter

Orbital moment sum rule for Au sites

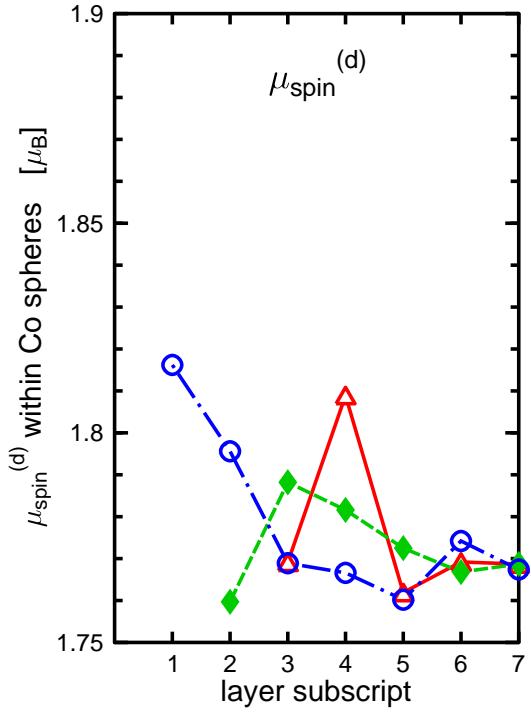
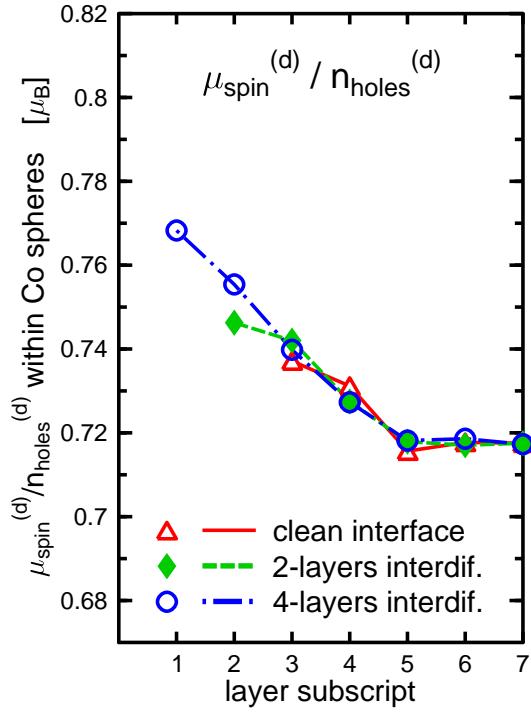
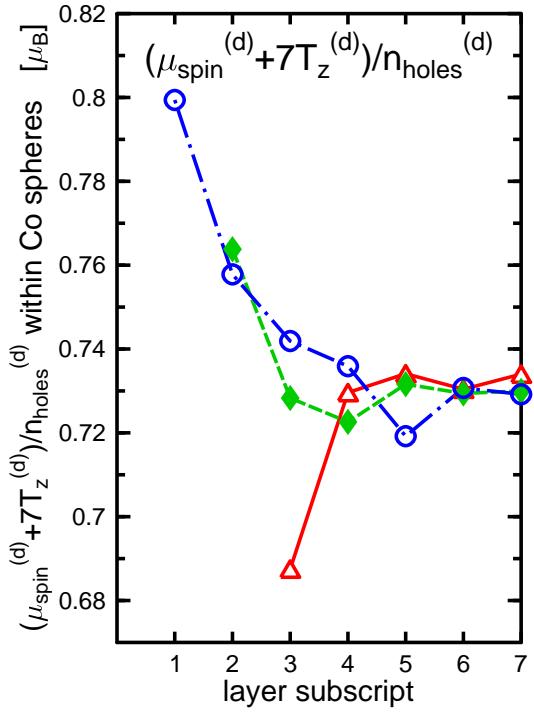


Orbital moment sum rule for Au sites

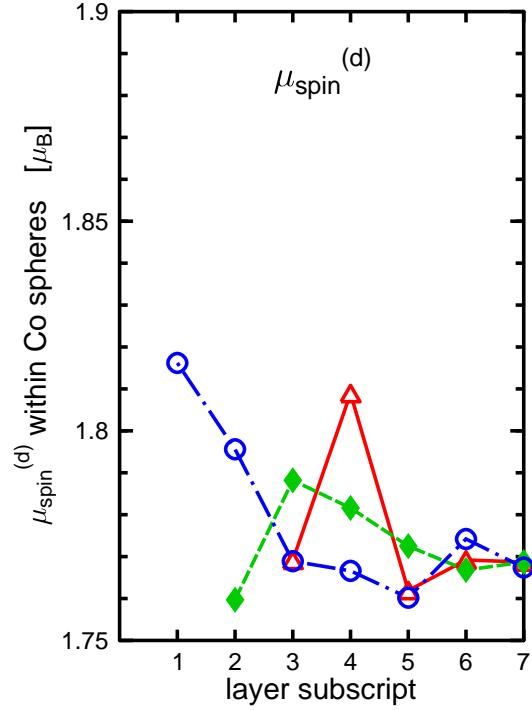
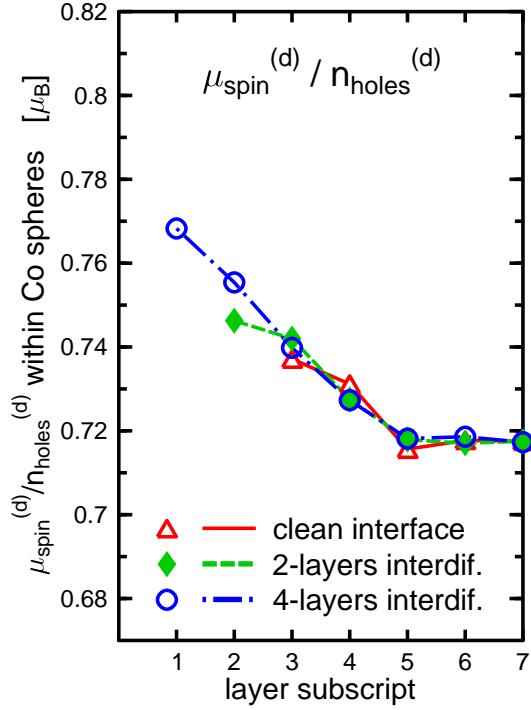
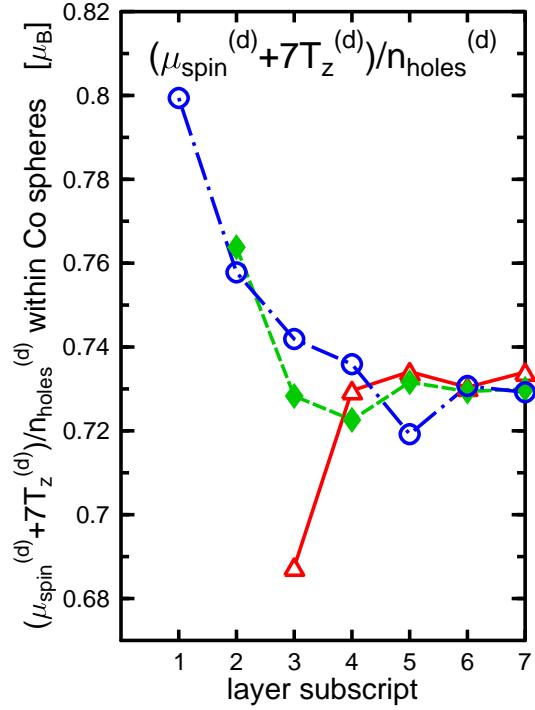


- $T_z^{(d)}$ contributes significantly

Spin moment sum rule for Co sites

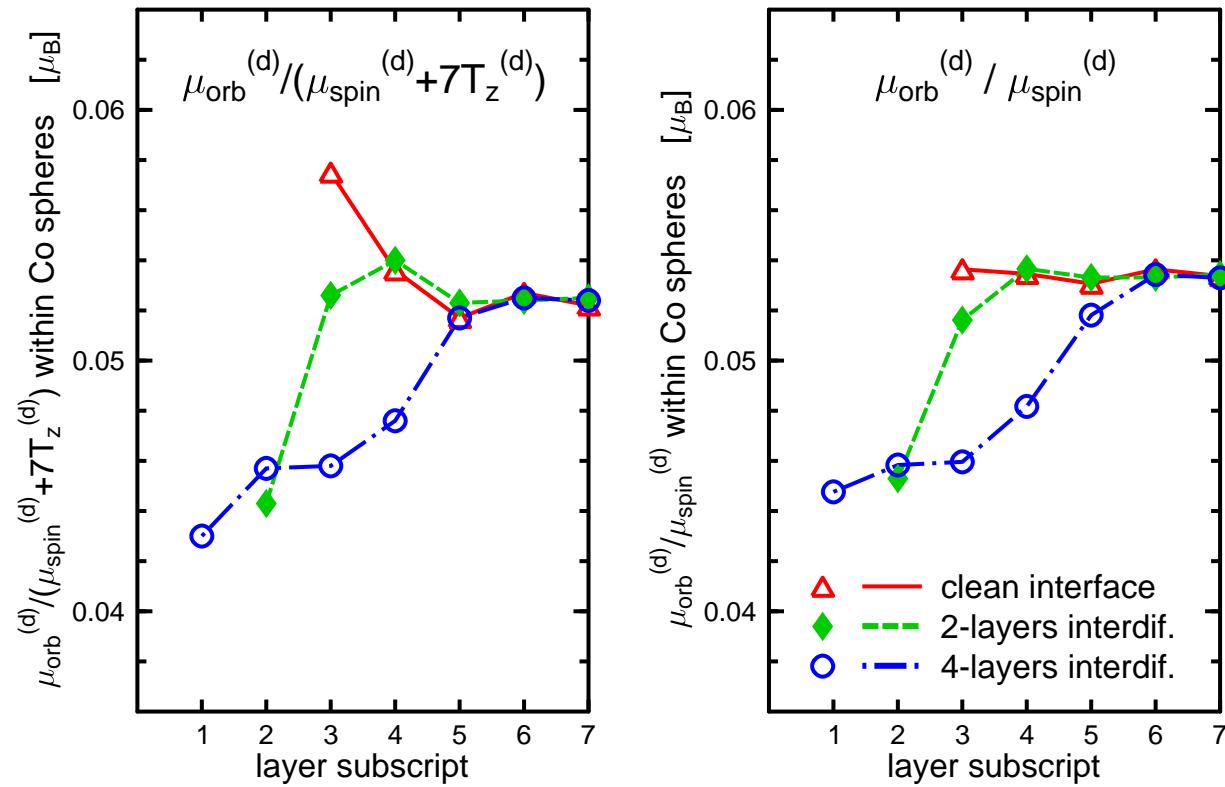


Spin moment sum rule for Co sites

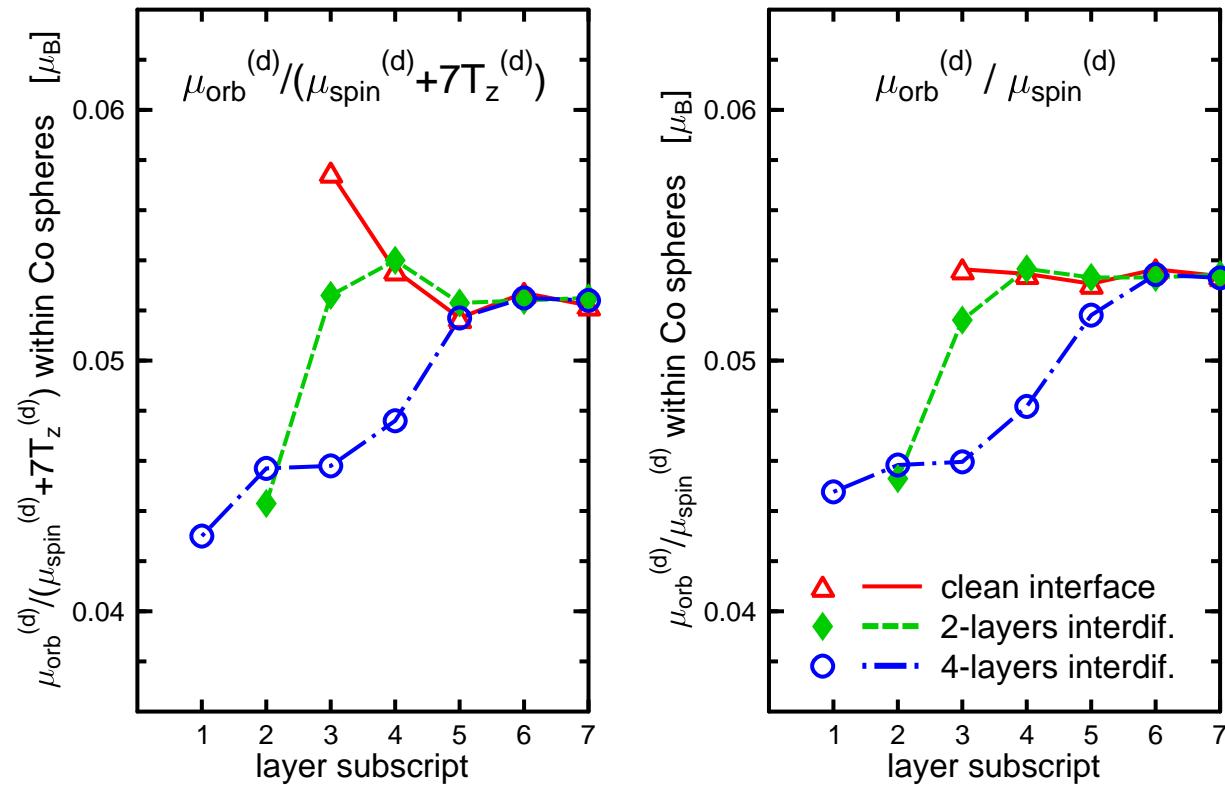


- Variations of $n_{\text{holes}}^{(d)}$ and $T_z^{(d)}$ matter quite a lot . . .

Orbital moment sum rule for Co sites



Orbital moment sum rule for Co sites

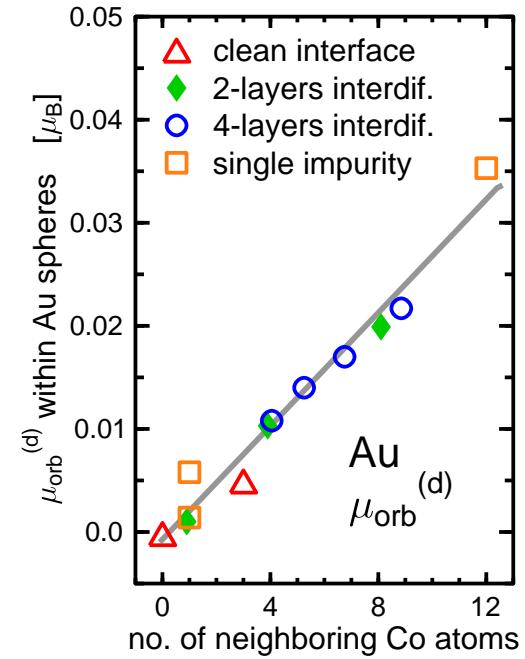
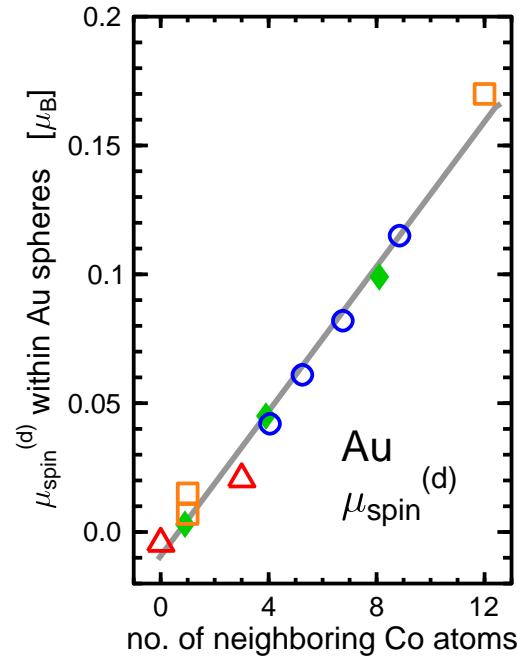
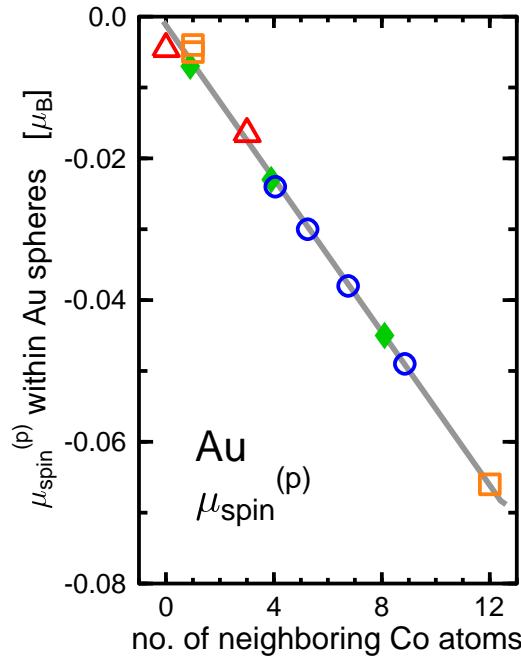


- $T_z^{(d)}$ contributes but not drastically

Dependence on coordination no.: Au

- $\mu_{spin}^{(p)}$, $\mu_{spin}^{(d)}$, and $\mu_{orb}^{(d)}$ at Au sites as function of the number of neighboring Co atoms

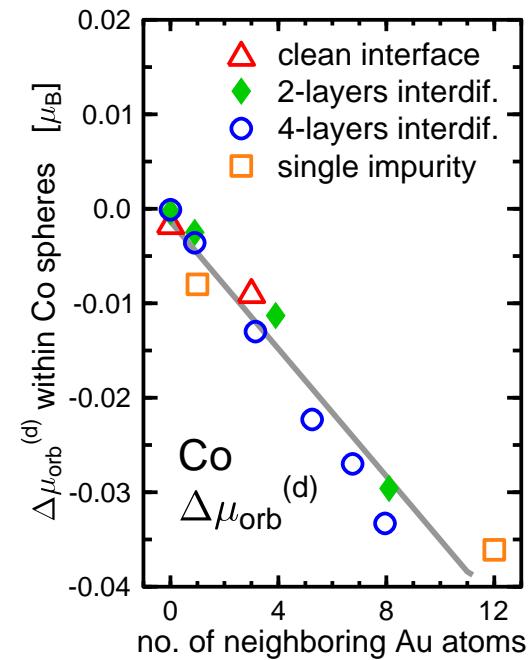
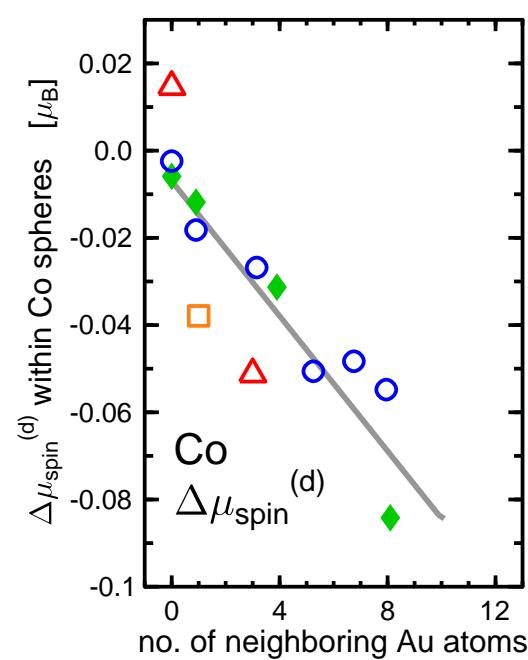
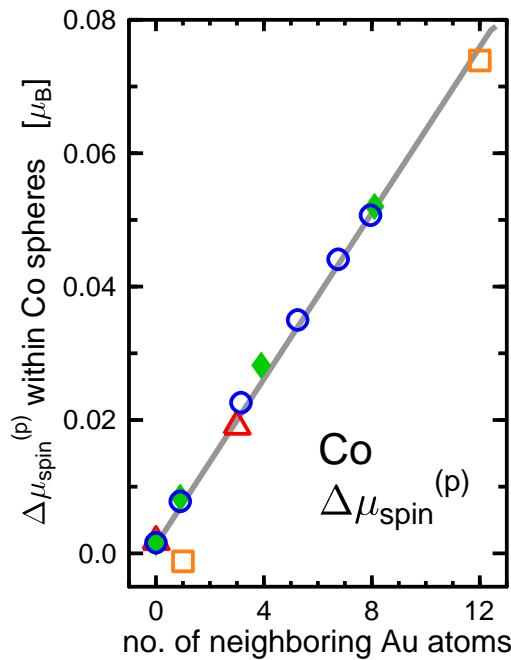
Magnetic moments of Au atoms in Au_4Co_{11} multilayer



Dependence on coordination no.: Co

- **Differences** between the true $\text{Au}_4\text{Co}_{11}$ multilayer and the auxiliary $\text{Co}_4\text{Co}_{11}$ model system: $\Delta\mu_{\text{spin}}^{(p)}$, $\Delta\mu_{\text{spin}}^{(d)}$, and $\Delta\mu_{\text{orb}}^{(d)}$ at Co sites as function of the number of neighboring Au atoms

Difference of magnetic moments of Co atoms in $\text{Au}_4\text{Co}_{11}$ multilayer and in a $\text{Co}_4\text{Co}_{11}$ model system



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 - Having Au atoms as neighbors suppresses magnetism