

# Fe: RSCAN vs PBE

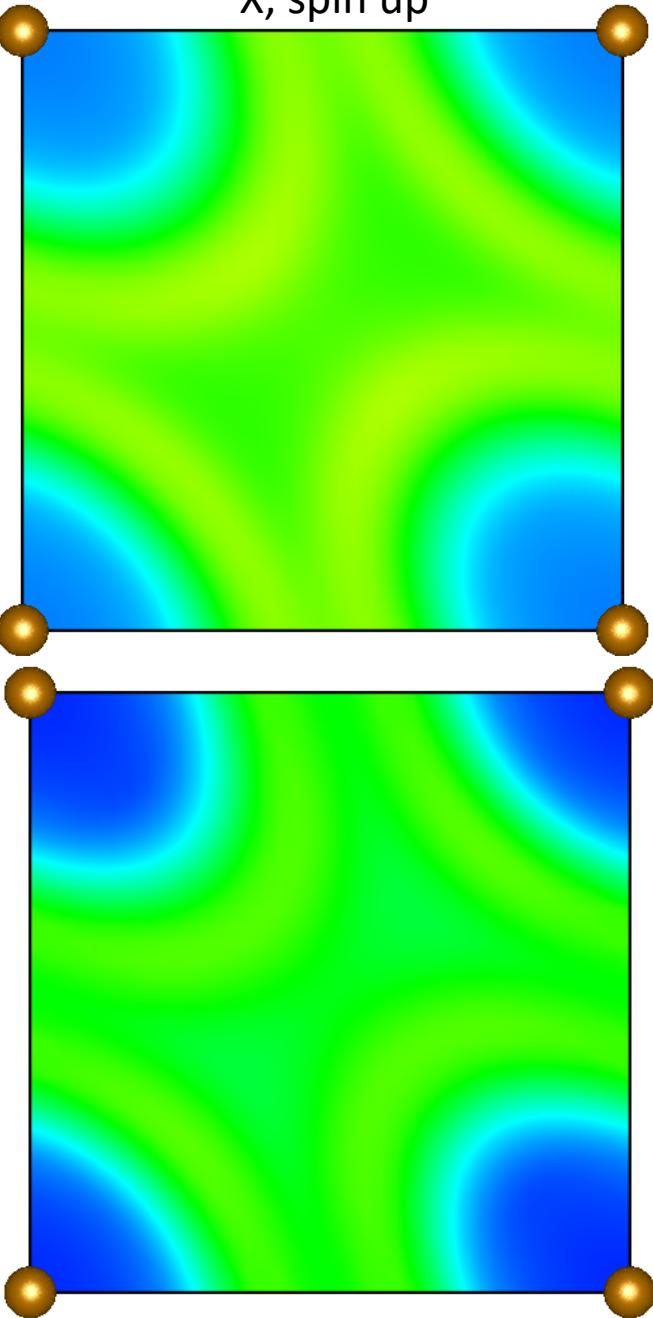
Lennart Gundelach

30.07.2019

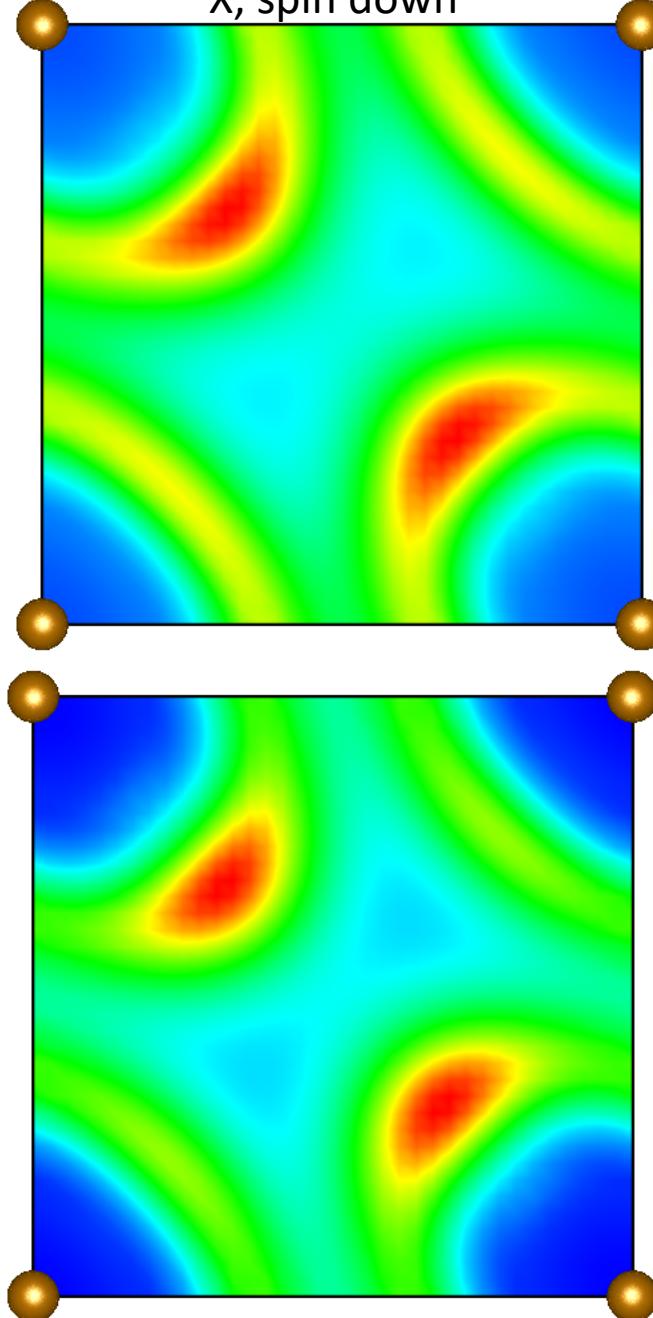
Oxford

Plane: (100), Distance from origin: 0d

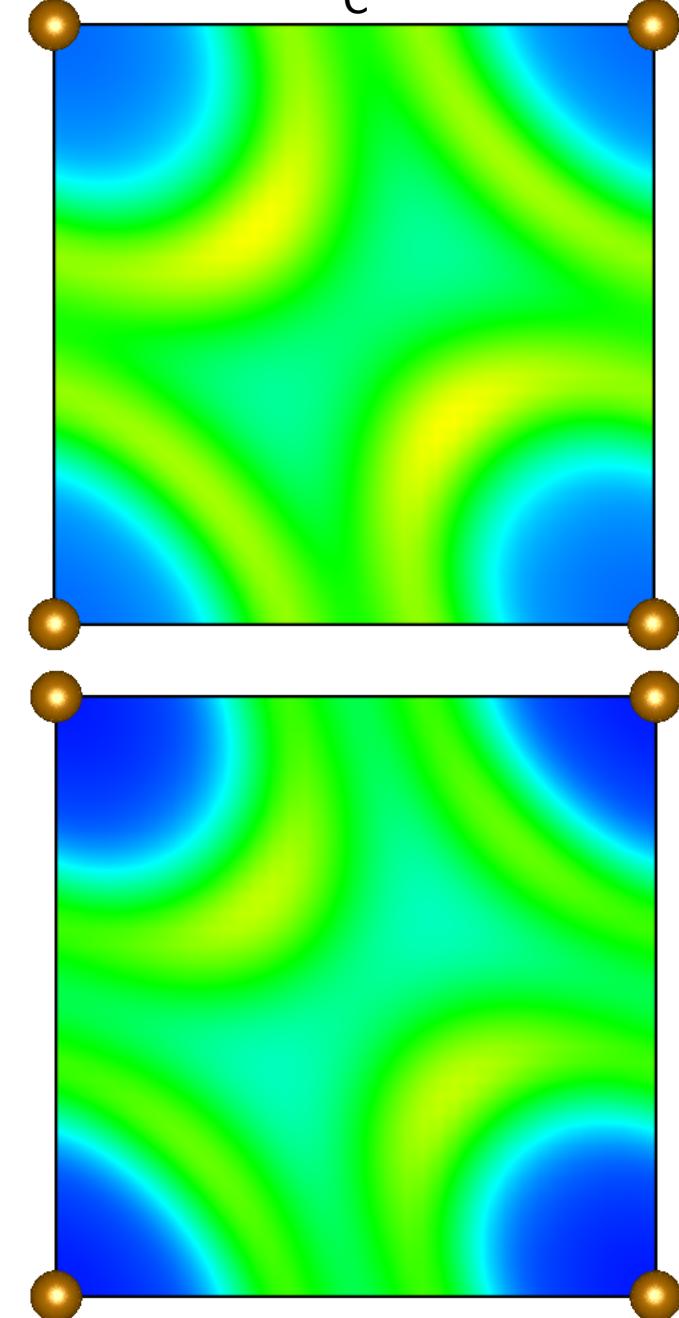
X, spin up



X, spin down

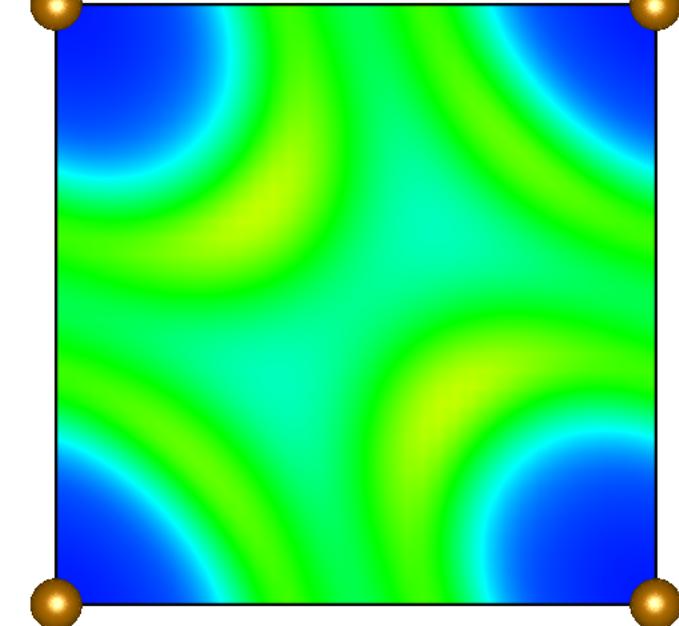
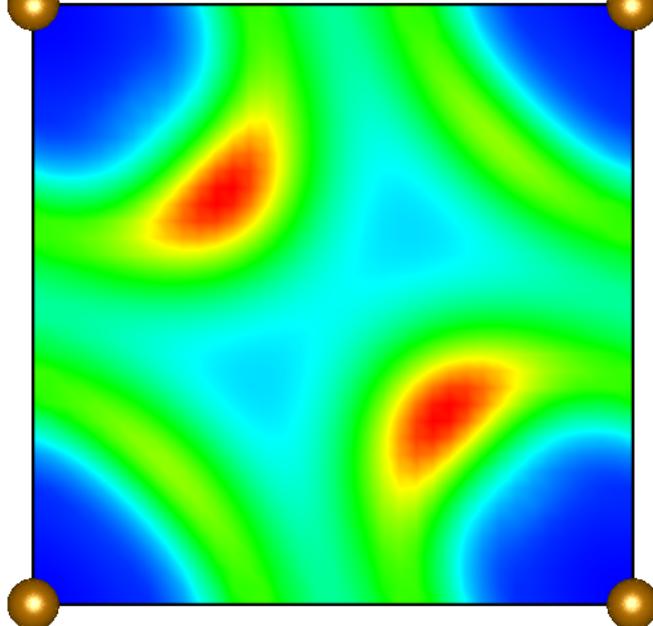
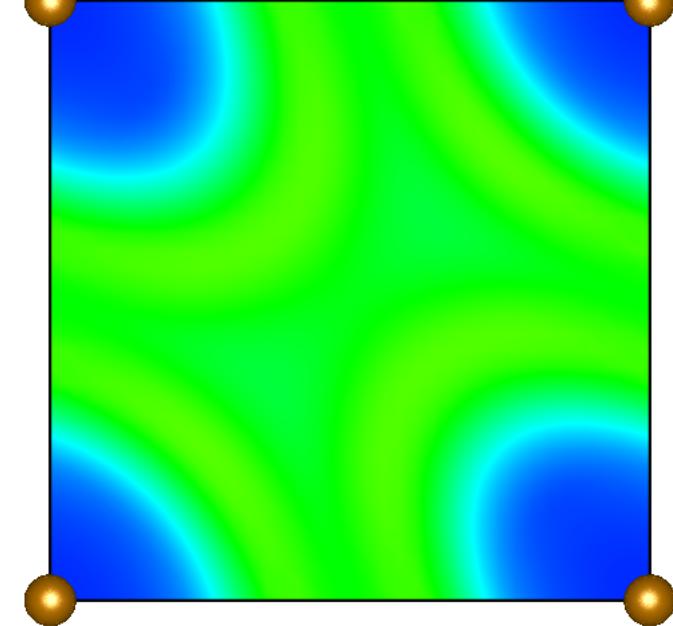


C



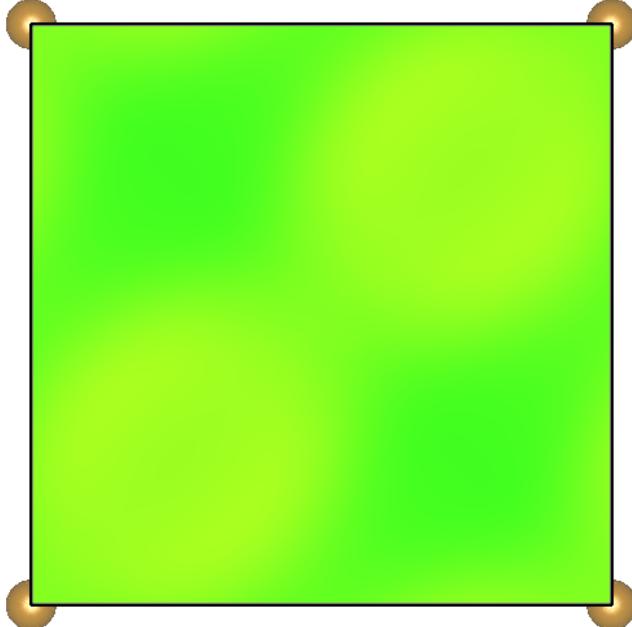
RSCAN

PBE

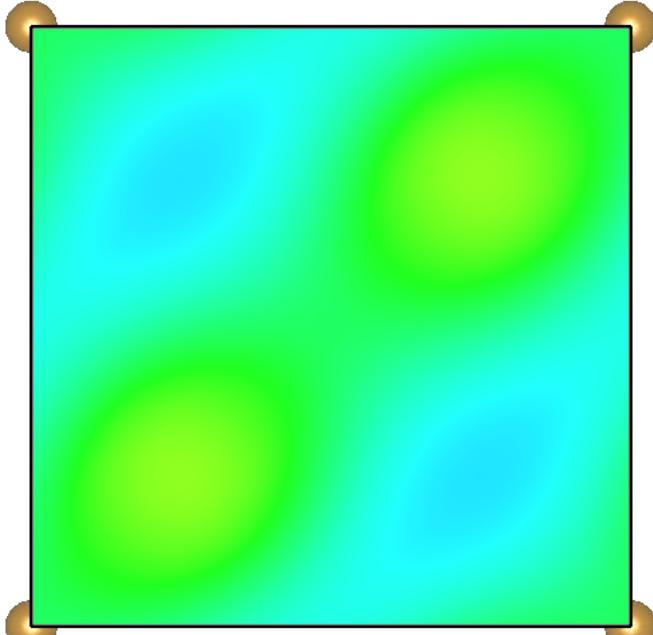


(100), 0.5d

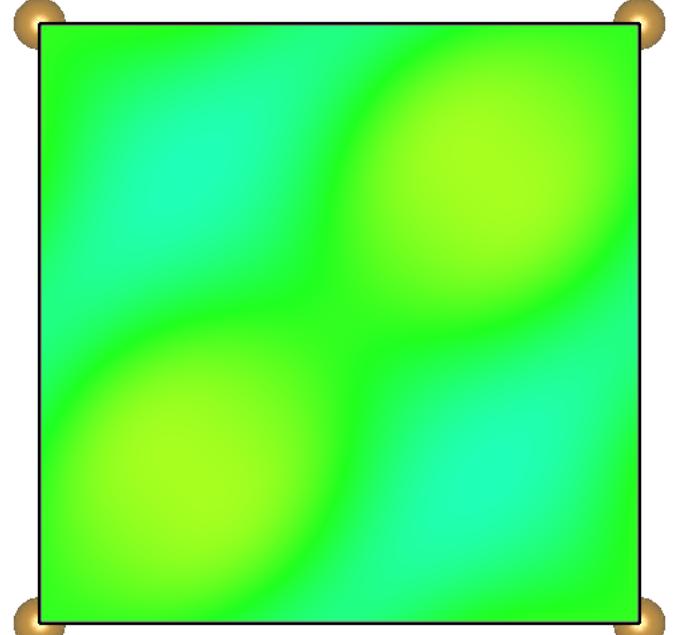
X, spin up



X, spin down

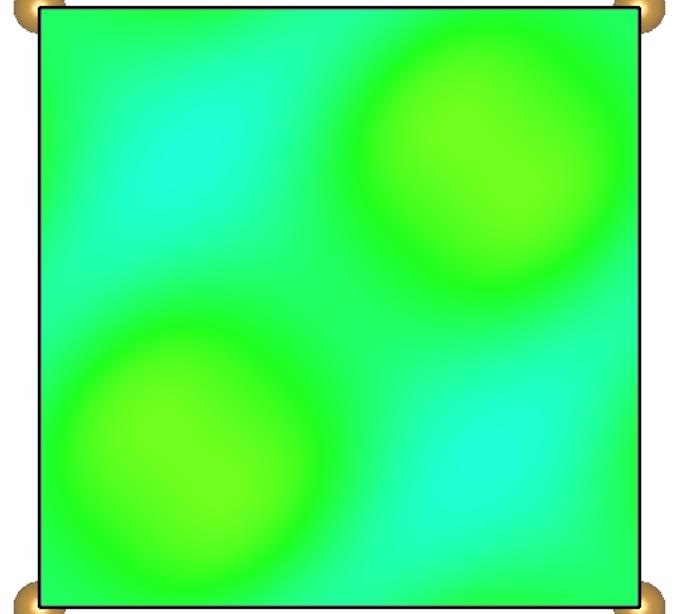
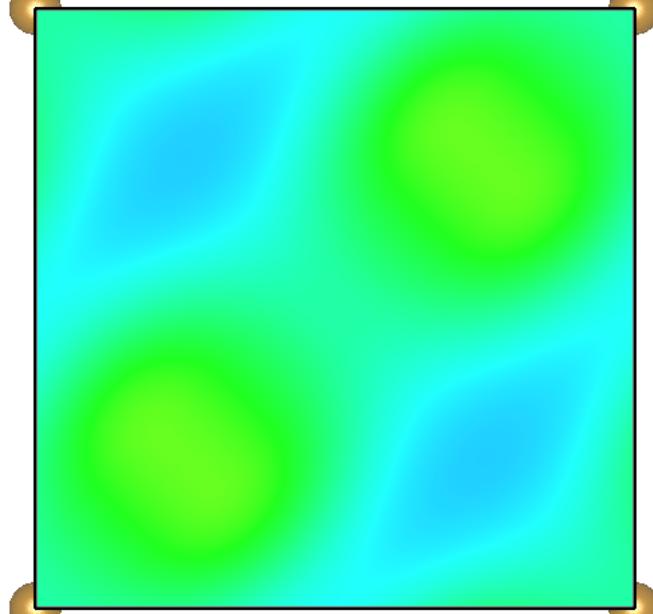
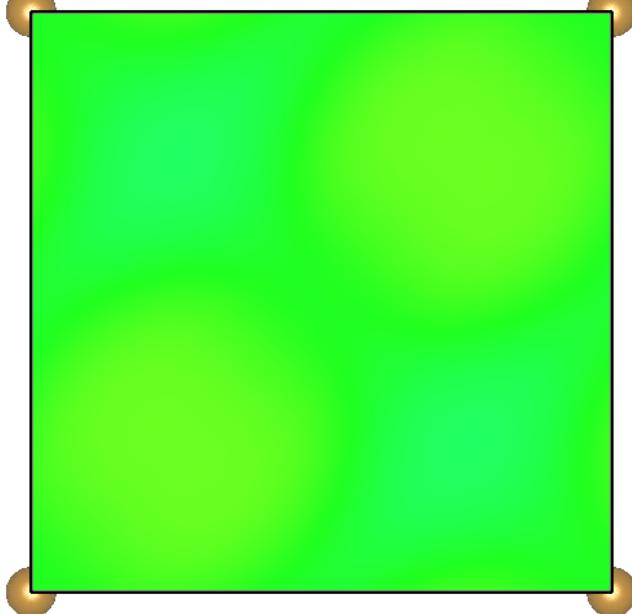


C



RSCAN

PBE



(110), 1d

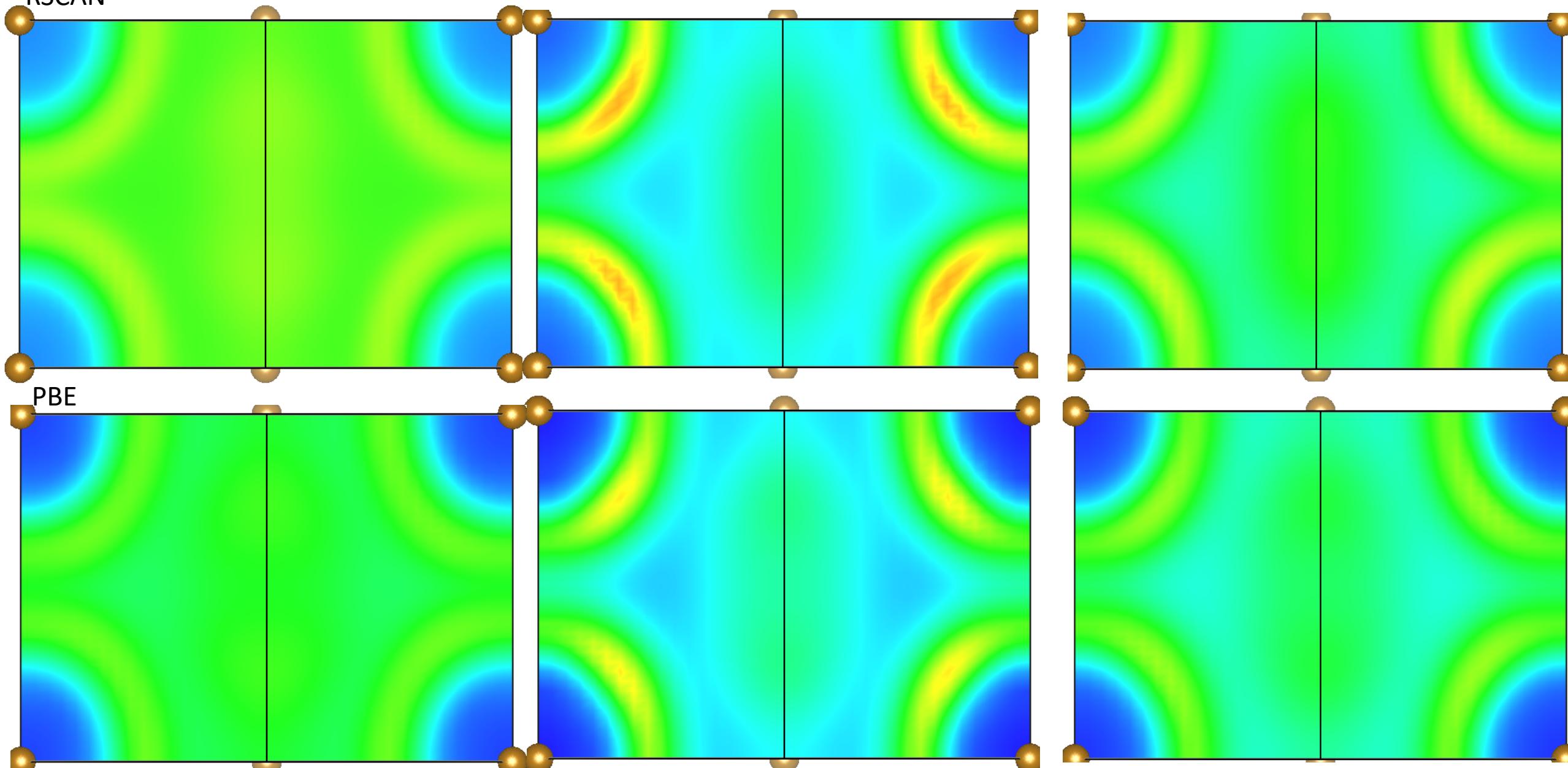
X, spin up

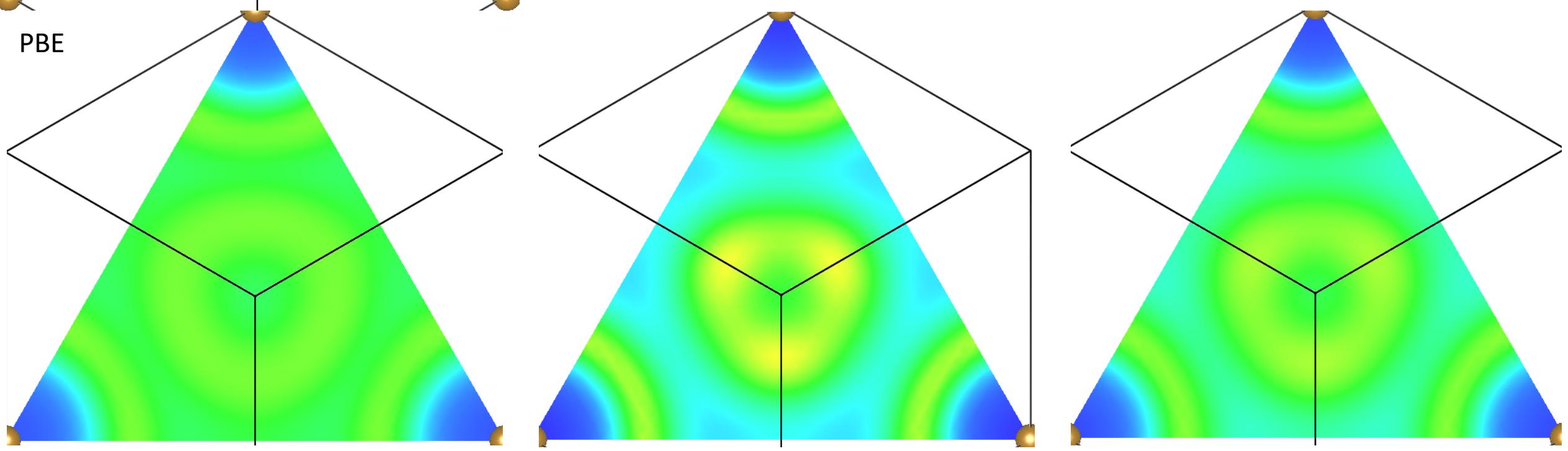
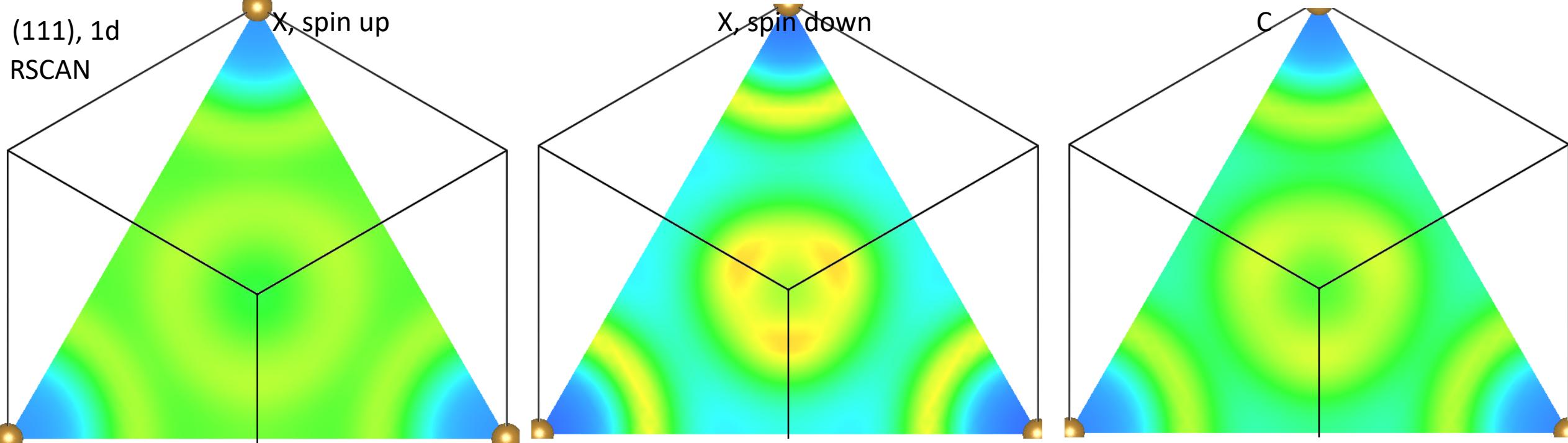
X, spin down

C

RSCAN

PBE





Data Set: 1  
Max: 2.28787214301088  
Min: 0.422850636576831  
Ave: 1.8168909159321909  
Mea: 1.96451729092958  
Data Set: 2  
Max: 3.41700698603114  
Min: 0.250320490609247  
Ave: 1.4911887607423806  
Mea: 1.3163134289218048  
Data Set: 2  
Max: 2.55726383142265  
Min: 0.354410905053774  
Ave: 1.6168236777098313  
Mea: 1.61553000232363

# Observations

- Shape of spatial patterns same in PBE and RSCAN
- Shape of spatial distributions same for X\_up, X\_down, C
- Magnitudes different for X\_up, X\_down, C
  - This is supported by summary statistics
  - see left hand side for alpha(1-3) in Fe using RSCAN

# Further Questions

- What do the spatial patterns of alpha tell us about local chemistry?
- How big is the pseudopotential region and does it correspond to the blue regions of very low alpha surrounding the atom sites?
- Why is X\_down noticeably large in iron, and can this trend be observed in other materials
- If the spatial distributions for alpha(1-3) are so similar, why are the frequency distributions so distinct.
  - i.e there must be more than just a shift in magnitude between alphas