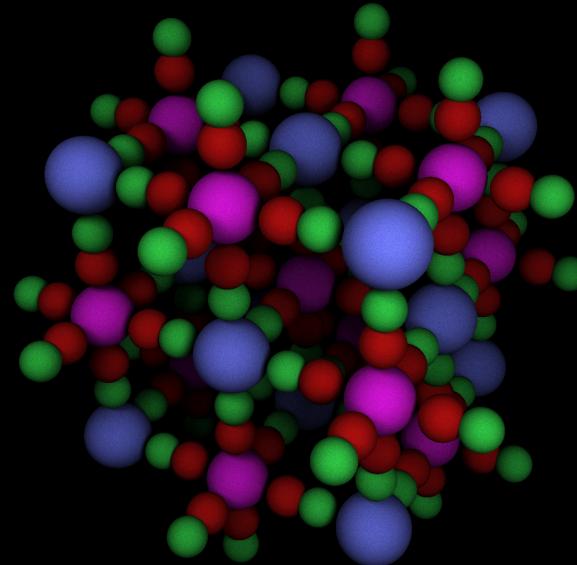


# Vacancy structure in Prussian blue analogues



Max Krummenacher

# Prussian blue analogues

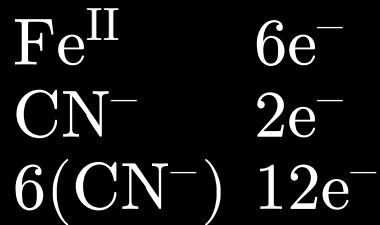


# Prussian blue analogues



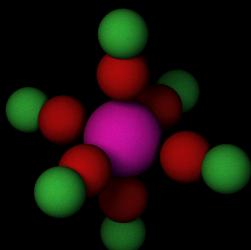
# Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]_{3/4}$

**18 VE rule (octahedral)**



# Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]_{3/4}$

18 VE rule (octahedral)



$\text{Fe}^{\text{III}}$

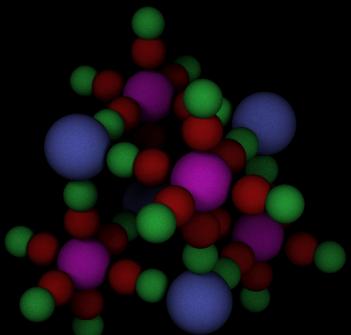
$\text{Fe}^{\text{II}}$

C

N

# Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]_{3/4}$

without charge neutrality



$\text{Fe}^{\text{III}}$

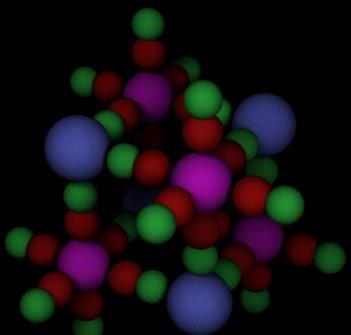
$\text{Fe}^{\text{II}}$

C

N

# Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]_{3/4}$

without charge neutrality

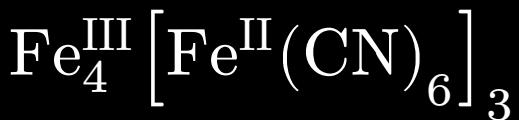


$\text{Fe}^{\text{III}}$

with charge neutrality



$\text{Fe}^{\text{III}}$

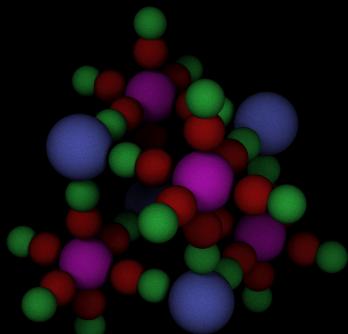


$\text{C}$

$\text{N}$

# Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]_{3/4}$

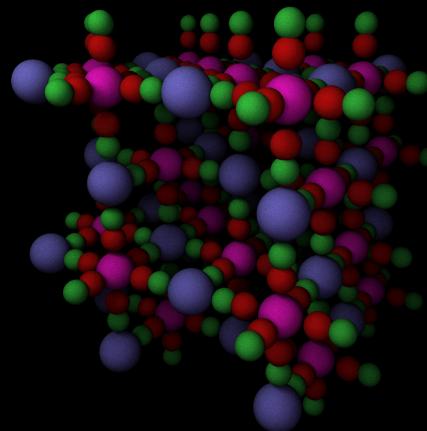
without charge neutrality



$\text{Fe}^{\text{III}}$

$\text{Fe}^{\text{II}}$

with charge neutrality

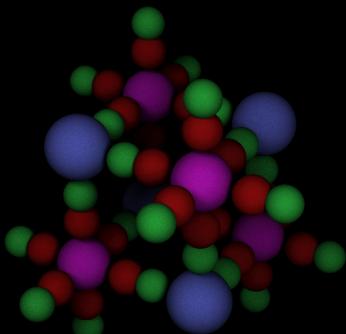


C

N

# Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]_{3/4}$

without charge neutrality



$\text{Fe}^{\text{III}}$

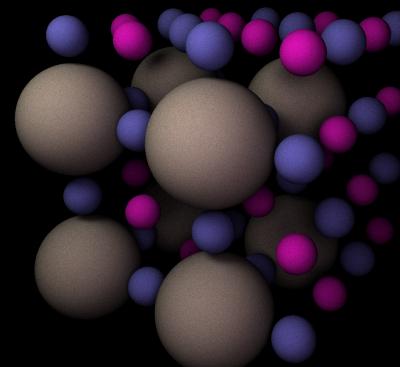
$\text{Fe}^{\text{II}}$

C

N

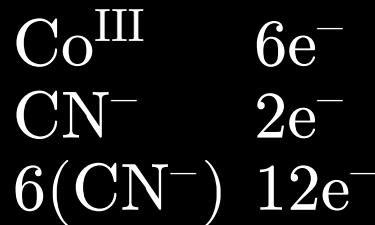
Vacancy

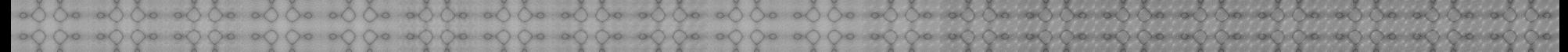
with charge neutrality



# Crystal structure of Mn $\left[\text{Co}(\text{CN})_6\right]_{2/3}$

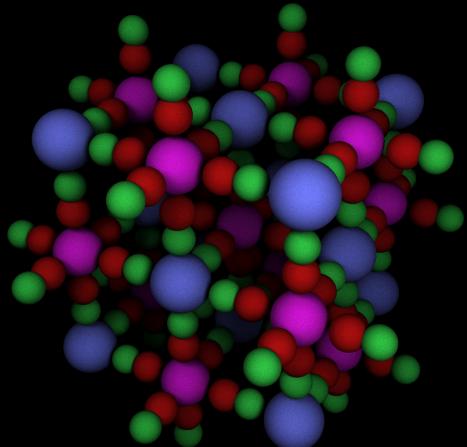
18 VE rule (octahedral)





# Crystal structure of $\text{Mn}[\text{Co}(\text{CN})_6]_{\frac{2}{3}}$

18 VE rule (octahedral)



Mn

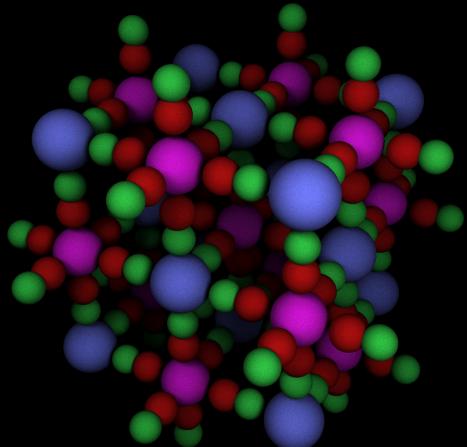
Co

C

N

# Crystal structure of $\text{Mn}\left[\text{Co}(\text{CN})_6\right]_{\frac{2}{3}}$

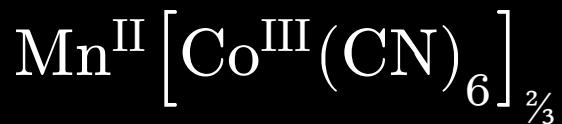
without charge neutrality



Mn

Co

with charge neutrality

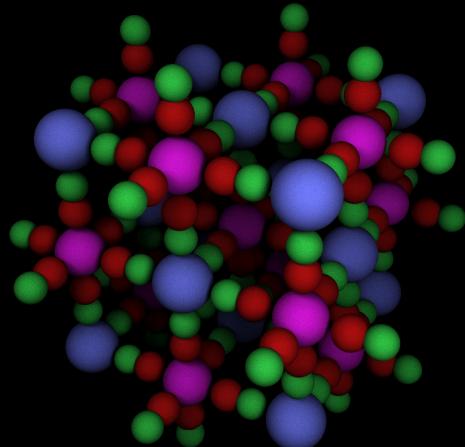


C

N

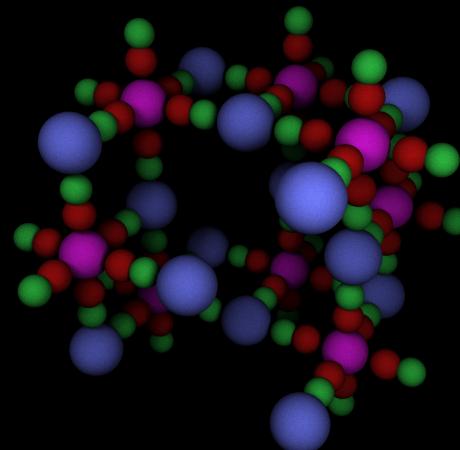
# Crystal structure of $\text{Mn}[\text{Co}(\text{CN})_6]_{\frac{2}{3}}$

without charge neutrality



Mn

with charge neutrality



Co

C

N

# Monte Carlo simulation

States

Hamiltonian

# Monte Carlo simulation

## States

- Grid with fixed Mn-ions

## Hamiltonian

# Monte Carlo simulation

## States

- Grid with fixed Mn-ions
- $\frac{2}{3}$  of cyanocobaltate positions filled

## Hamiltonian

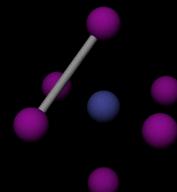
# Monte Carlo simulation

## States

- Grid with fixed Mn-ions
- $\frac{2}{3}$  of cyanocobaltate positions filled

## Hamiltonian

- nearest neighbor  $J_1$



Co

Mn

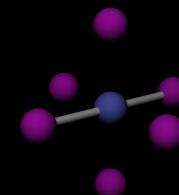
# Monte Carlo simulation

## States

- Grid with fixed Mn-ions
- $\frac{2}{3}$  of cyanocobaltate positions filled

## Hamiltonian

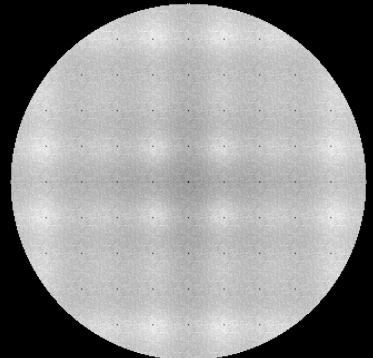
- nearest neighbor  $J_1$
- next nearest neighbor  $J_2$



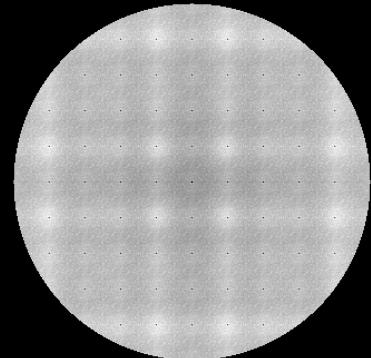
Co

Mn

# Diffraction

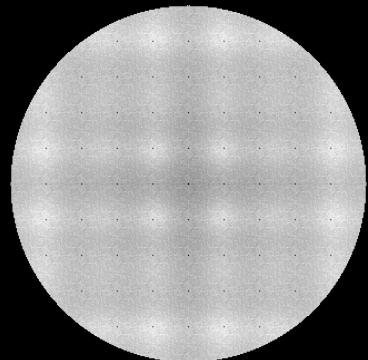


$\frac{J_1}{J_2} = 0.4$   
high  $T$

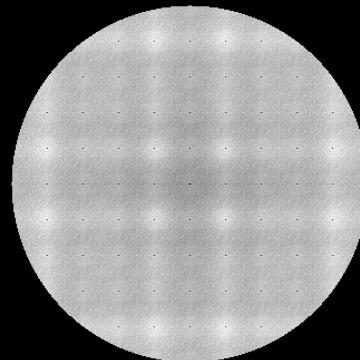


$\frac{J_1}{J_2} = 4.8$   
high  $T$

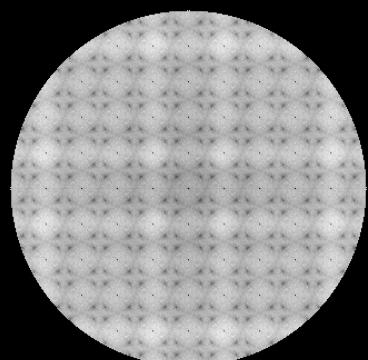
# Diffraction



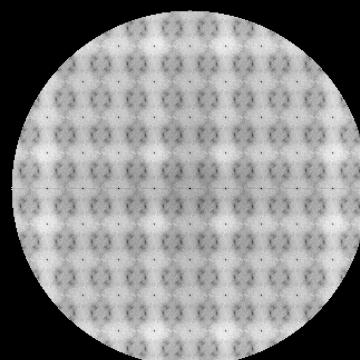
$\frac{J_1}{J_2} = 0.4$   
high  $T$



$\frac{J_1}{J_2} = 4.8$   
high  $T$



$\frac{J_1}{J_2} = 0.4$   
low  $T$



$\frac{J_1}{J_2} = 4.8$   
low  $T$

Thank you for your attention

