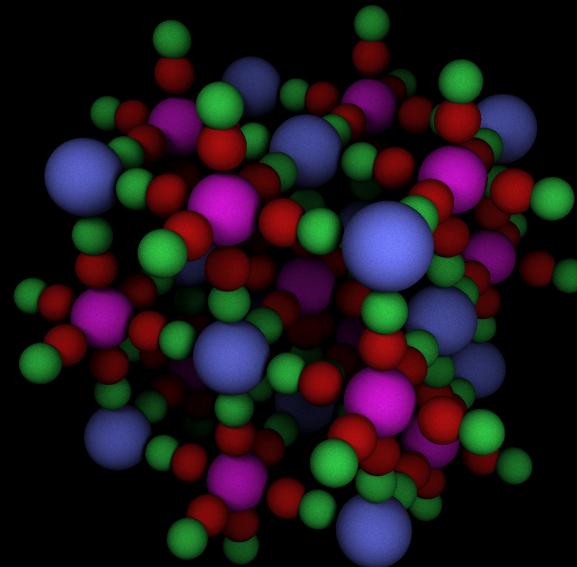


Vacancy structure in Prussian blue analogues



Max Krummenacher

Prussian blue analogues



Prussian blue analogues



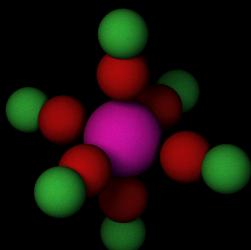
Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]_{3/4}$

18 VE rule (octahedral)



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

18 VE rule (octahedral)



Fe^{III}

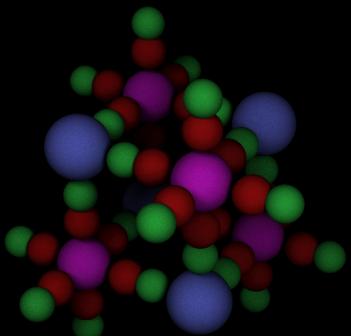
Fe^{II}

C

N

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

without charge neutrality



Fe^{III}

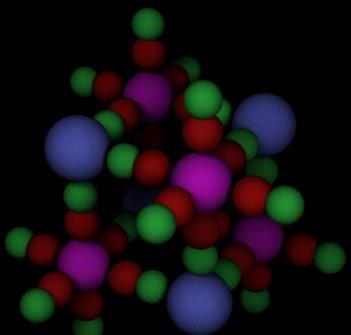
Fe^{II}

C

N

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

without charge neutrality

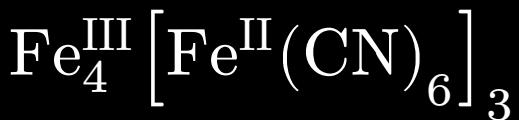


Fe^{III}

with charge neutrality



Fe^{III}

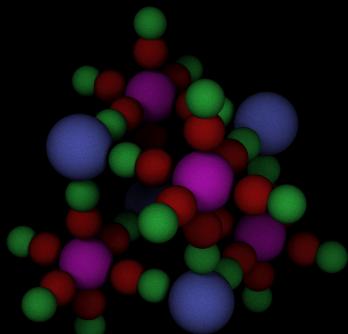


C

N

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

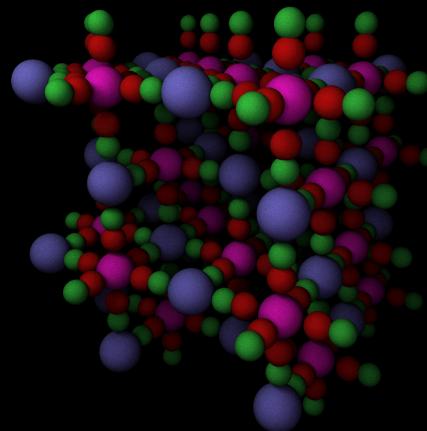
without charge neutrality



Fe^{III}

Fe^{II}

with charge neutrality

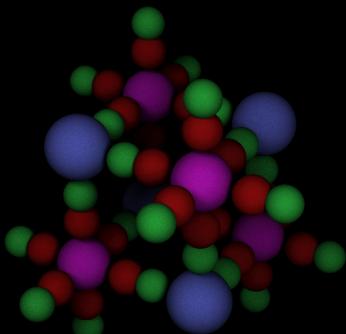


C

N

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

without charge neutrality



Fe^{III}

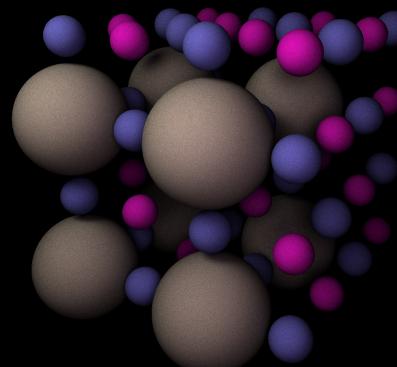
Fe^{II}

C

N

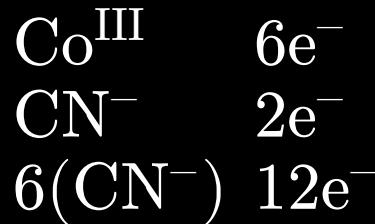
Vacancy

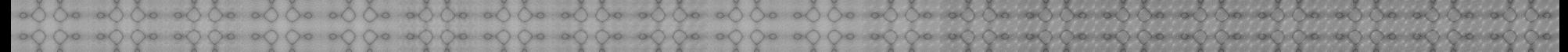
with charge neutrality



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

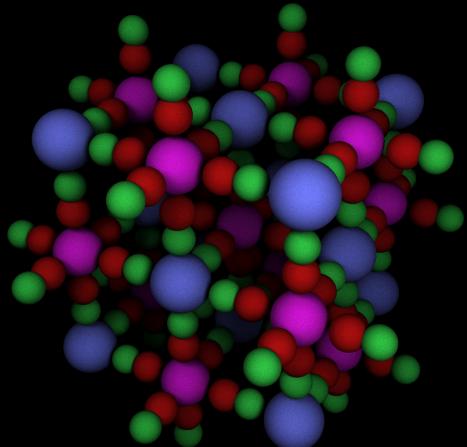
18 VE rule (octahedral)





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

18 VE rule (octahedral)



Mn

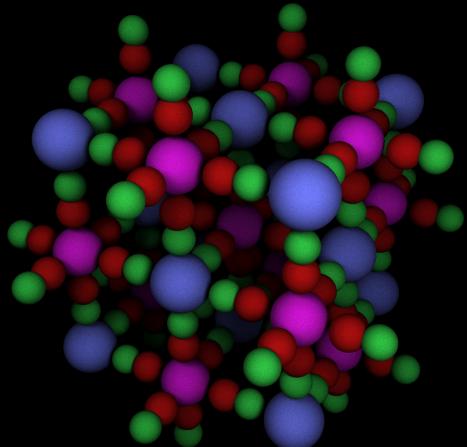
Co

C

N

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

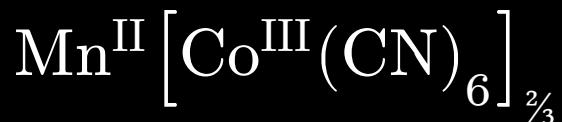
without charge neutrality



Mn

Co

with charge neutrality

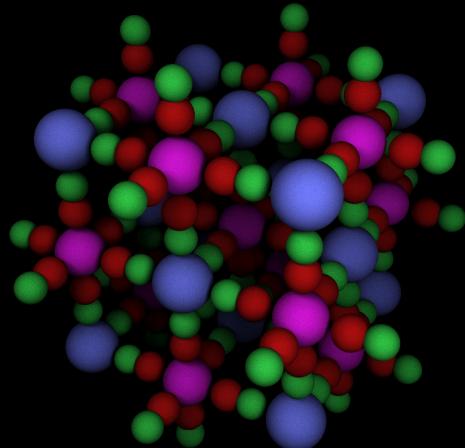


C

N

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

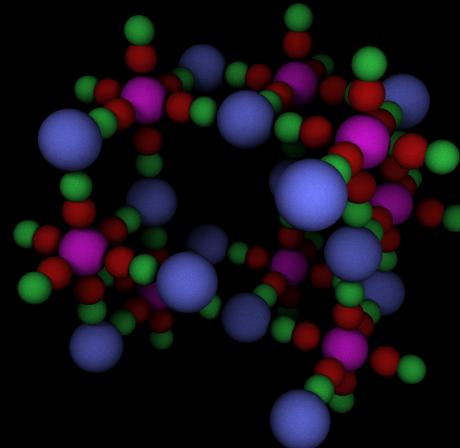
without charge neutrality



Mn

Co

with charge neutrality



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

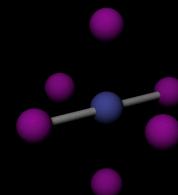
Monte Carlo simulation

States

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

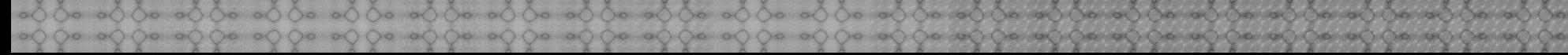
Hamiltonian

- nearest neighbor J_1
- next nearest neighbor J_2

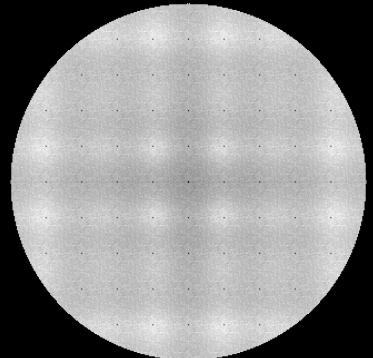


Co

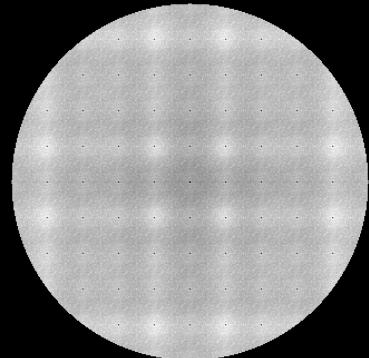
Mn



Diffraction

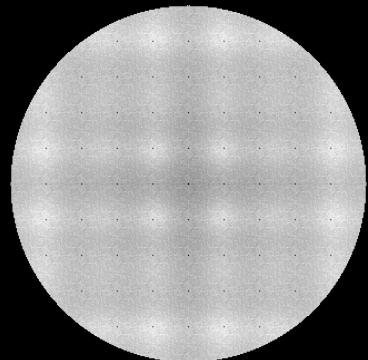


$\frac{J_1}{J_2} = 0.4$
high T

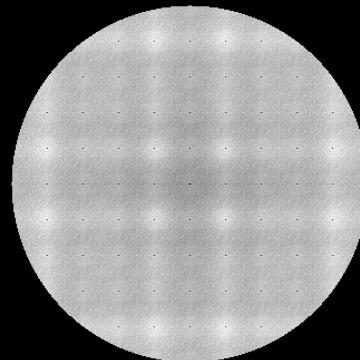


$\frac{J_1}{J_2} = 4.8$
high T

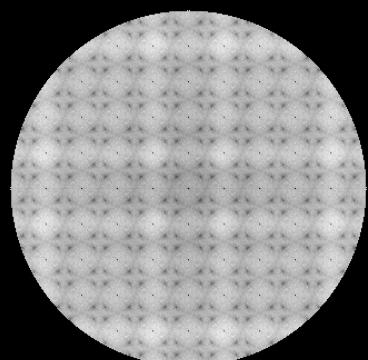
Diffraction



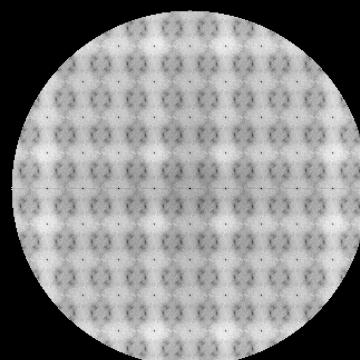
$\frac{J_1}{J_2} = 0.4$
high T



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

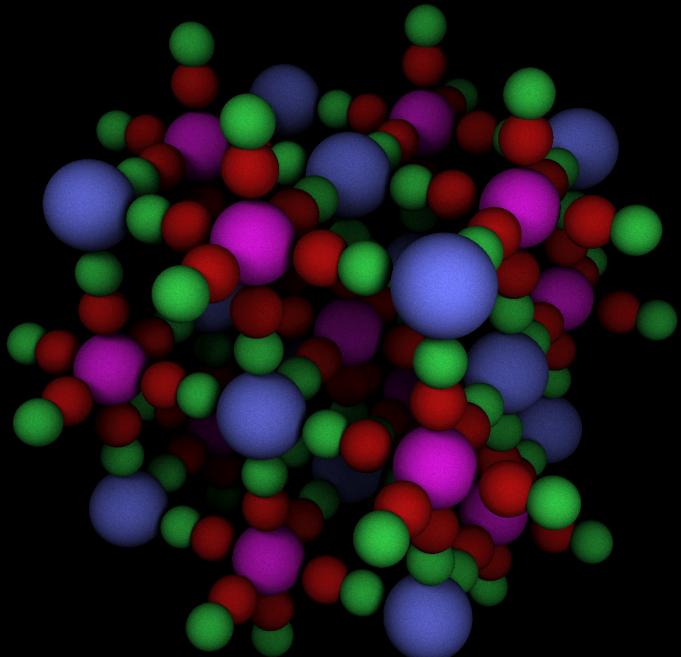


$\frac{J_1}{J_2} = 0.4$
low T



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

Thank you for your attention!



under supervision of

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Disordered Materials