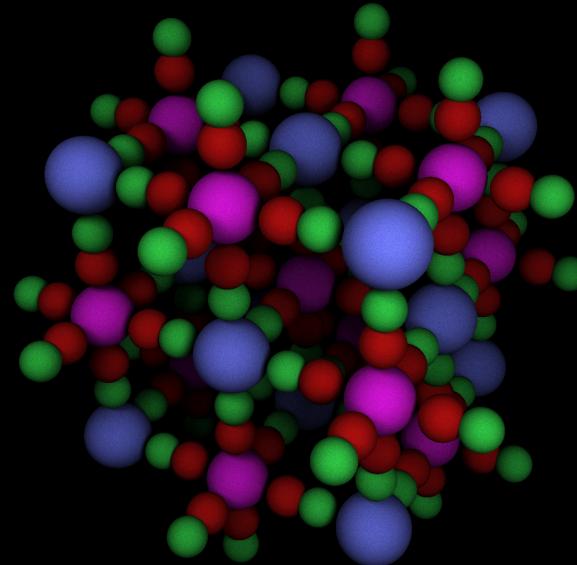


Vacancy structure in prussian blue analogues



Max Krummenacher

Prussian blue analogues



Prussian blue analogues



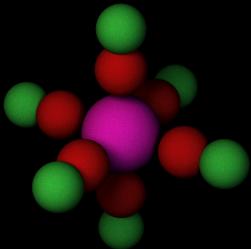
Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]$

18 VE rule (octahedral)



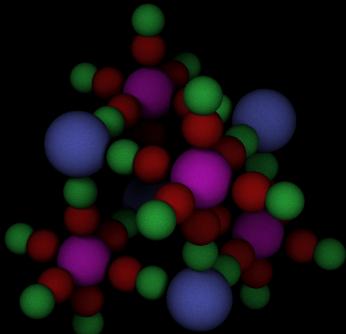
Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]$

18 VE rule (octahedral)



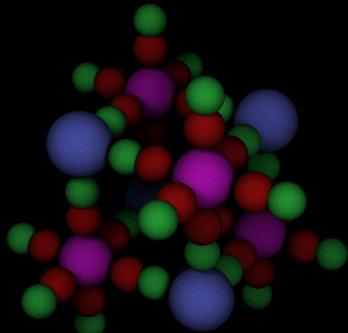
Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]$

without charge neutrality

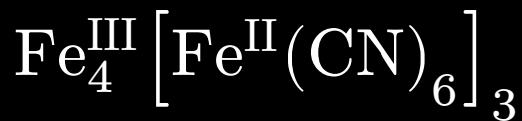


Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]$

without charge neutrality

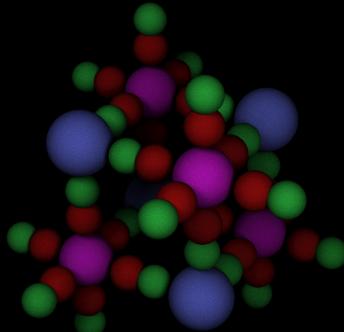


with charge neutrality

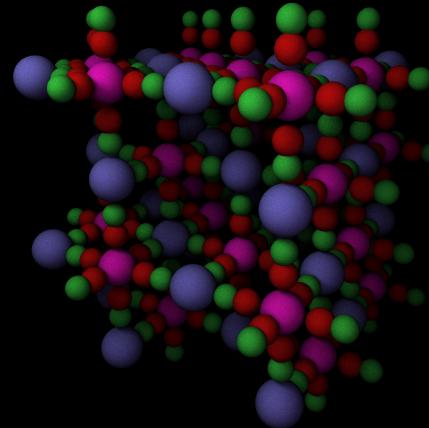


Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]$

without charge neutrality

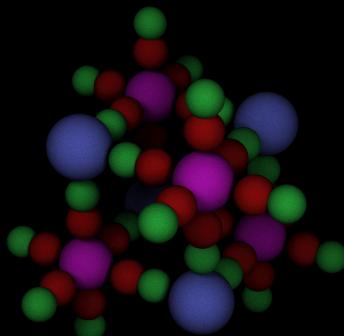


with charge neutrality

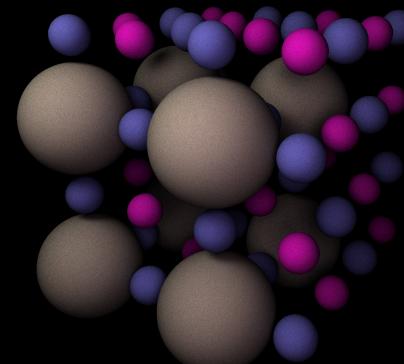


Crystal structure of $\text{Fe}[\text{Fe}(\text{CN})_6]$

without charge neutrality

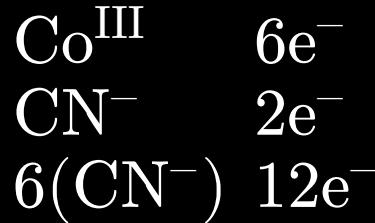


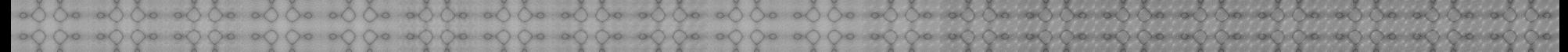
with charge neutrality



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

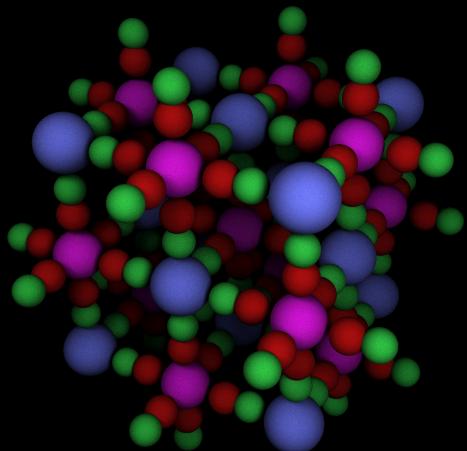
18 VE rule (octahedral)





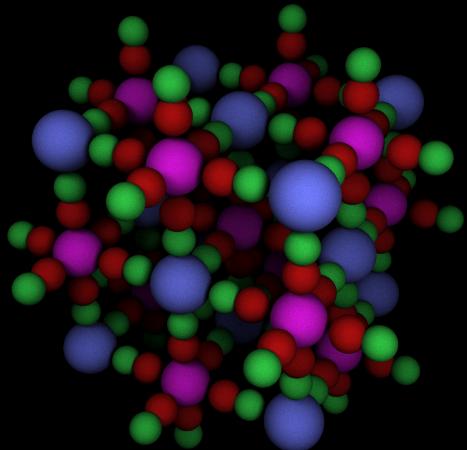
Crystal structure of Mn $\left[\text{Co}(\text{CN})_6\right]$

18 VE rule (octahedral)

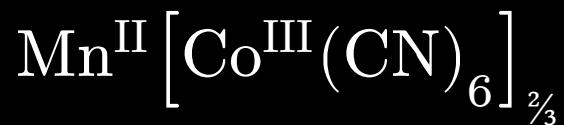


Crystal structure of Mn $\left[\text{Co}(\text{CN})_6\right]$

without charge neutrality

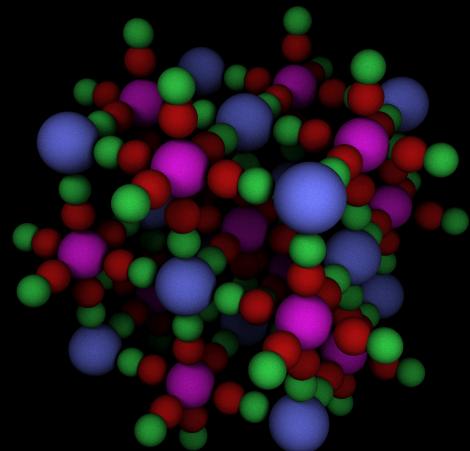


with charge neutrality

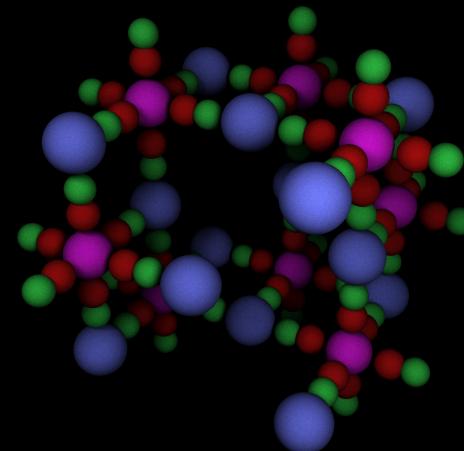


Crystal structure of Mn $\left[\text{Co}(\text{CN})_6\right]$

without charge neutrality



with charge neutrality



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

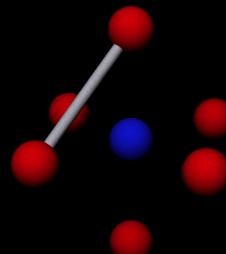
Monte Carlo simulation

States

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

Hamiltonian

- nearest neighbor J_1



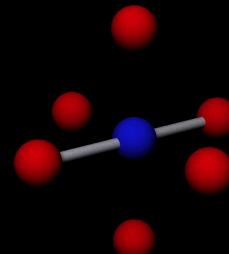
Monte Carlo simulation

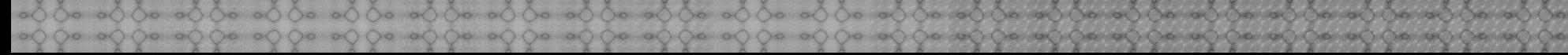
States

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

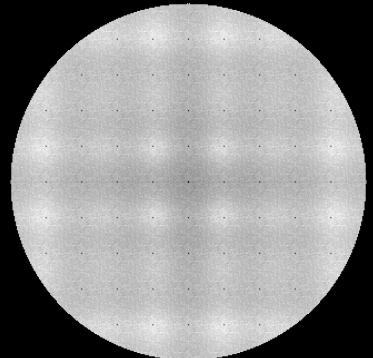
Hamiltonian

- nearest neighbor J_1
- next nearest neighbor J_2

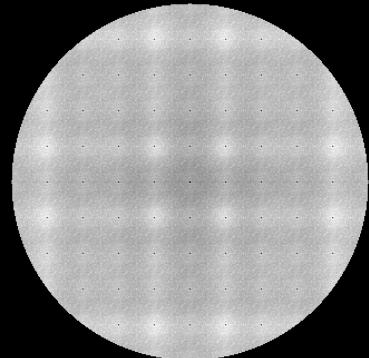




Diffraction

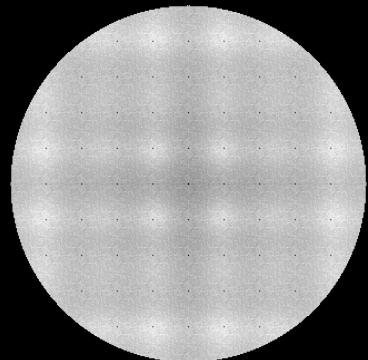


$\frac{J_1}{J_2} = 0.4$
high T

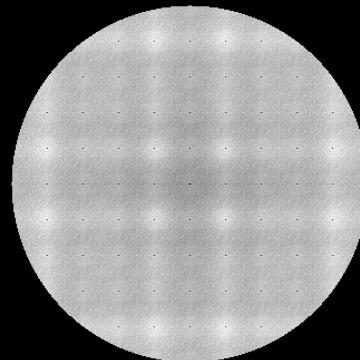


$\frac{J_1}{J_2} = 4.8$
high T

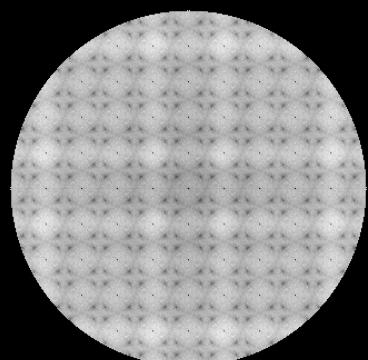
Diffraction



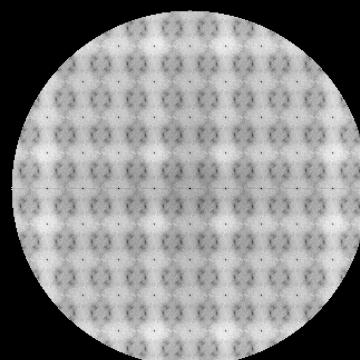
$\frac{J_1}{J_2} = 0.4$
high T



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



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



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