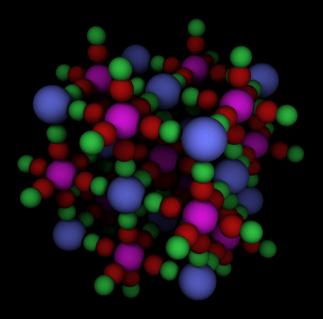
# Vacancy structure in manganese hexakiscyanocobaltate

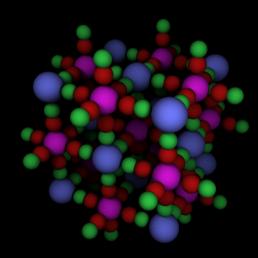


Max Krummenacher

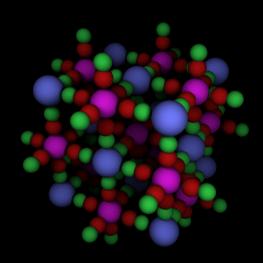
# 18 VE rule (octahedral symmetry)

$$egin{array}{lll} {
m Co^{III}} & 6{
m e^-} \\ {
m CN^-} & 2{
m e^-} \\ 6({
m CN^-}) & 12{
m e^-} \end{array}$$

18 VE rule (octahedral symmetry)



#### without charge neutrality



#### with charge neutrality

 $\mathrm{Co}^{\mathrm{III}}$ 

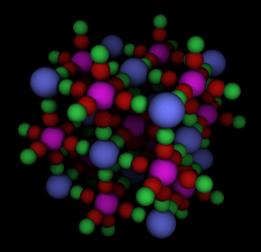
 $CN^{-}$ 

$$\left[\mathrm{Co^{III}(CN)}_{6}\right]^{-3}$$

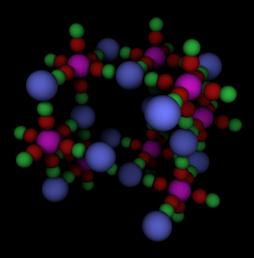
 $m Mn^{II}$ 

$$\mathrm{Mn^{II}} \left[ \mathrm{Co^{III}(CN)}_{6} \right]_{\frac{2}{3}}$$

without charge neutrality



with charge neutrality



#### **Monte Carlo simulation**

## 

# Results