

Temperature dependent EXAFS analysis of structural disorder in the

using Monte Carlo methods and evolutionary algorithm

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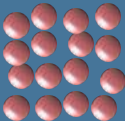
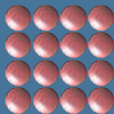
Reverse Monte Carlo Genetic algorithm



Reverse Monte Carlo
Genetic algorithm



**Disorder in $\text{Co}_3\text{O}_2\text{BO}_3$
seems to be relevant**



Reverse Monte Carlo
Genetic algorithm



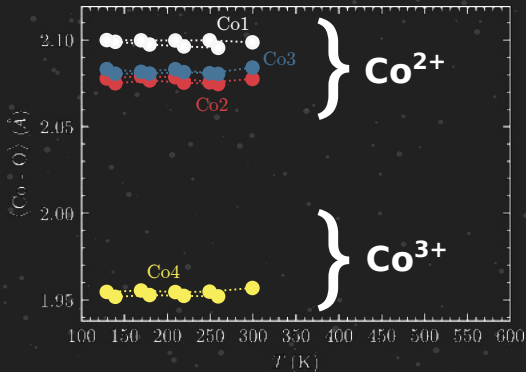
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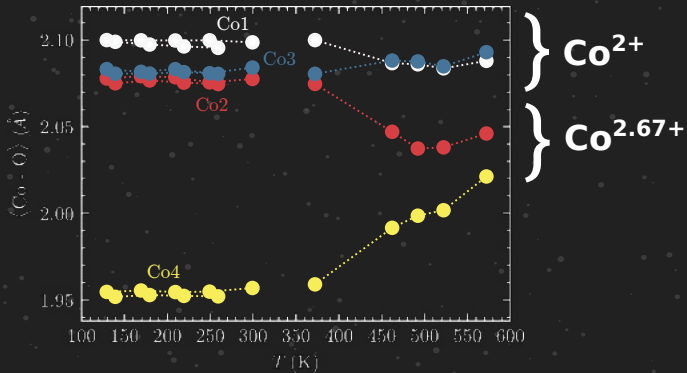
**Charge rearrangement
at high temperatures**



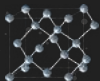
Single crystal X-ray diffraction



Single crystal X-ray diffraction

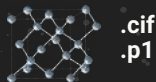


Evolutionary Algorithm for EXAFS analysis

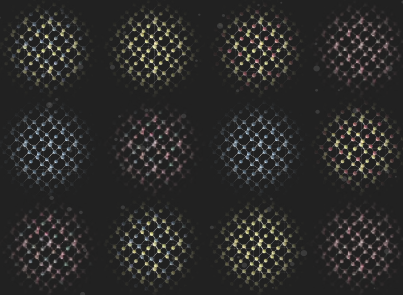
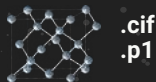


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Evolutionary Algorithm for EXAFS analysis

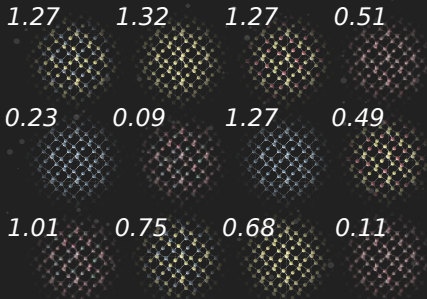
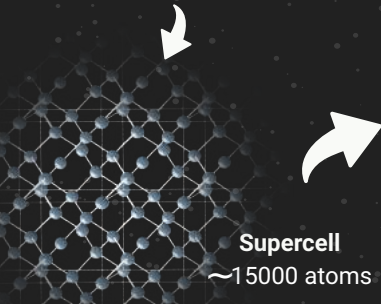
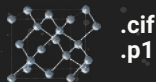


Evolutionary Algorithm for EXAFS analysis



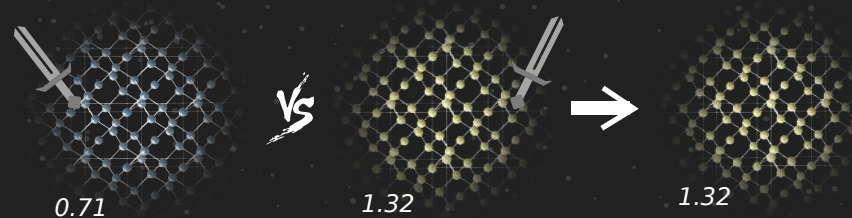
Population
32 individuals

Evolutionary Algorithm for EXAFS analysis



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Evolutionary Algorithm for EXAFS analysis



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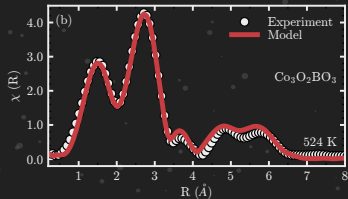
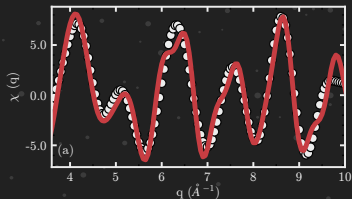


Evolutionary Algorithm for EXAFS analysis

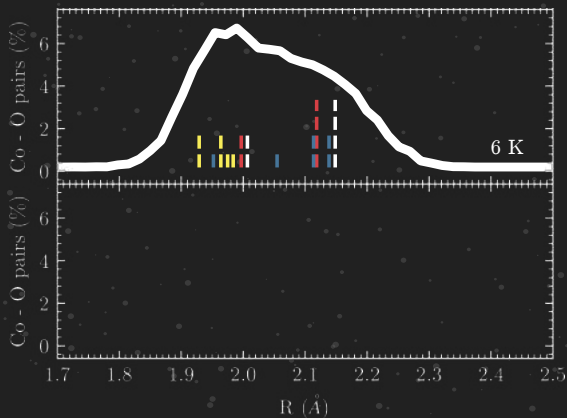
vs ♥ ☠
~5000 gen.

Evolutionary Algorithm for EXAFS analysis

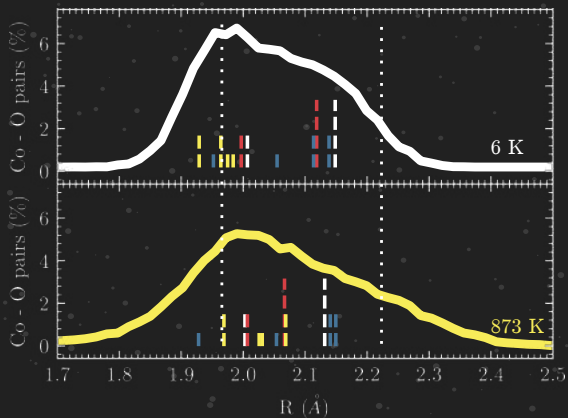
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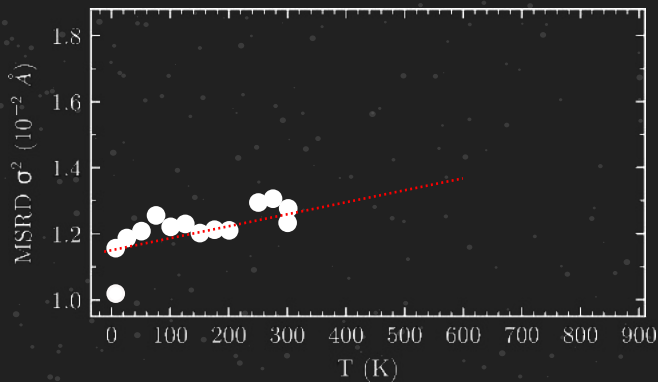
Pair distribution function (PDF)



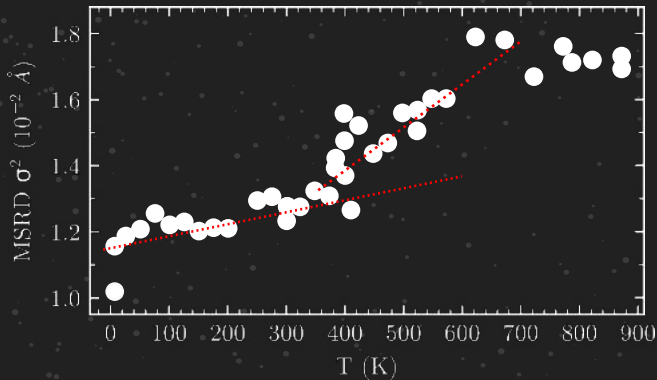
Pair distribution function (PDF)



Standard deviation (EXAFS Debye-Waller factor)



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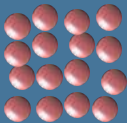
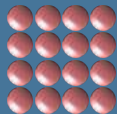
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