



Enabling efficient electrochemical hydrogen peroxide through geometrical nanoparticle size effects

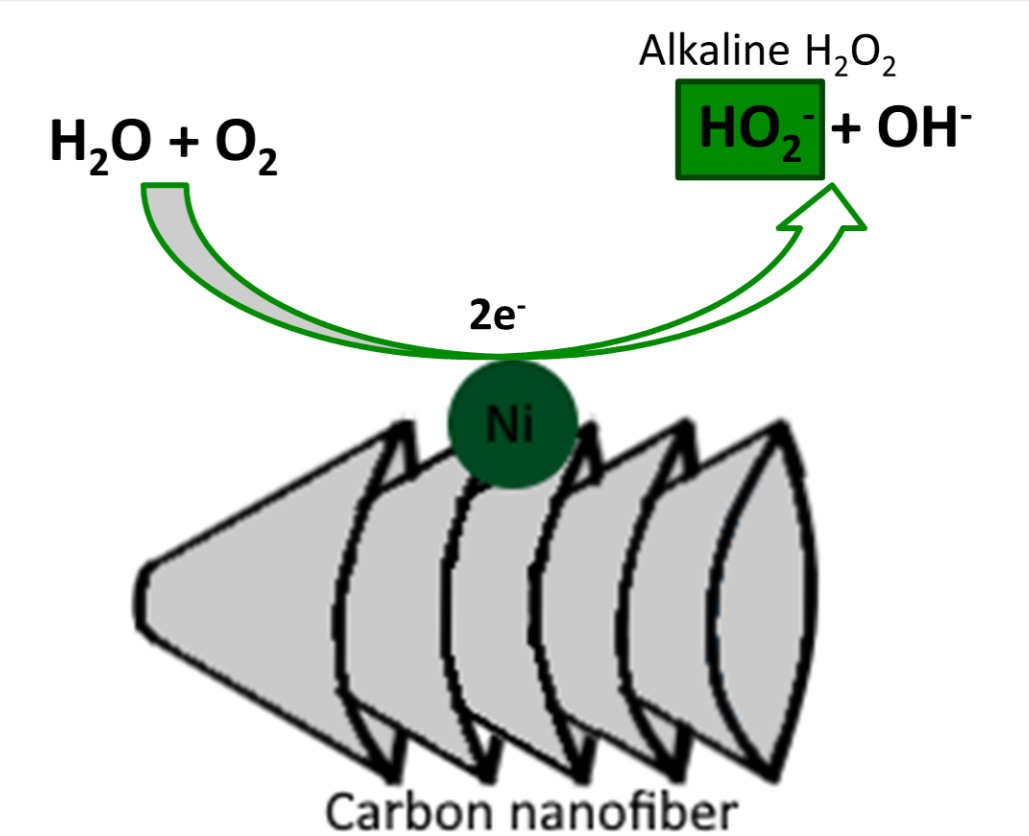
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Background

- Current hydrogen peroxide production produces 1.1 million tons of CO₂
- Electrochemical production from oxygen and water is possible but better catalysts (cathode) are required to increase electron efficiency and reduce overpotential, lowering energy use
- Non-noble transition metal nanoparticles can be an effective catalyst

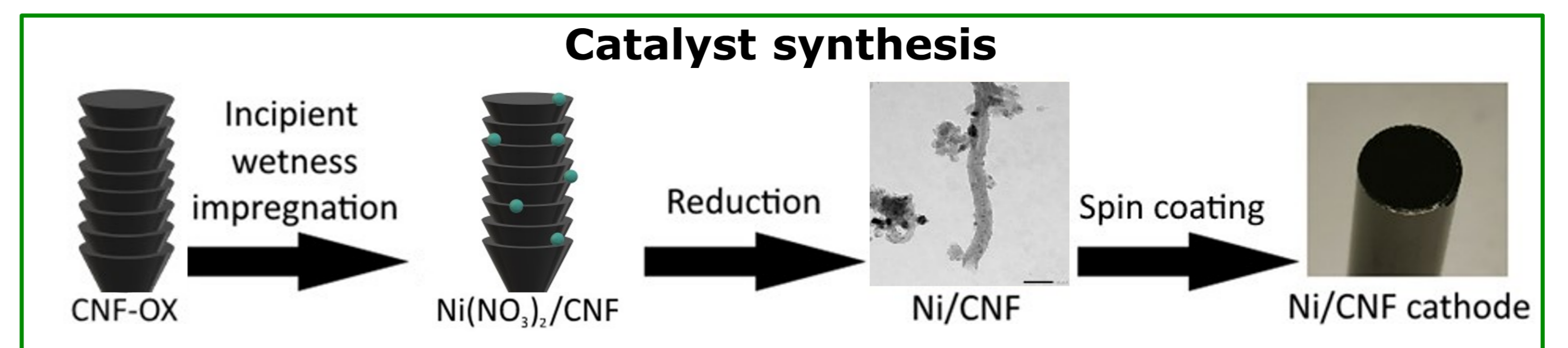
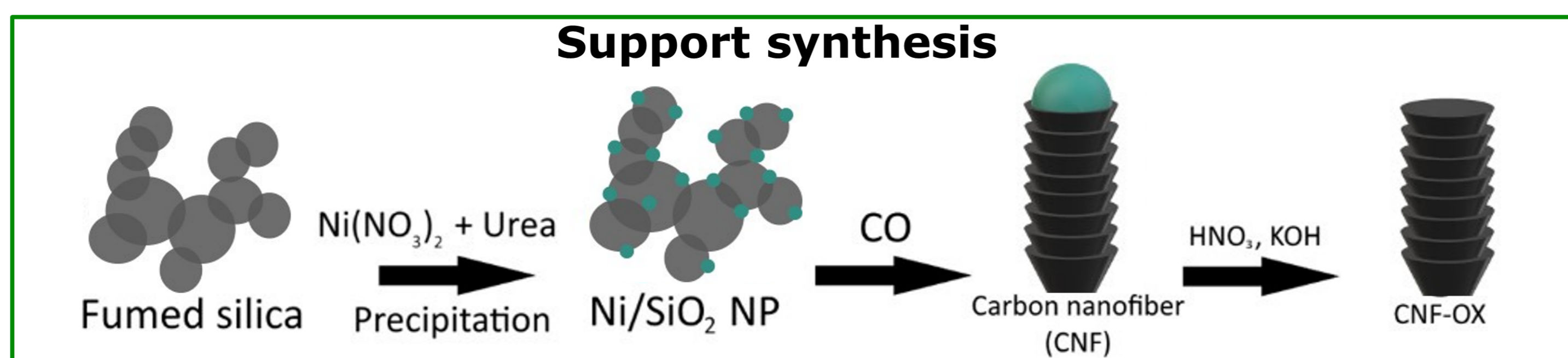
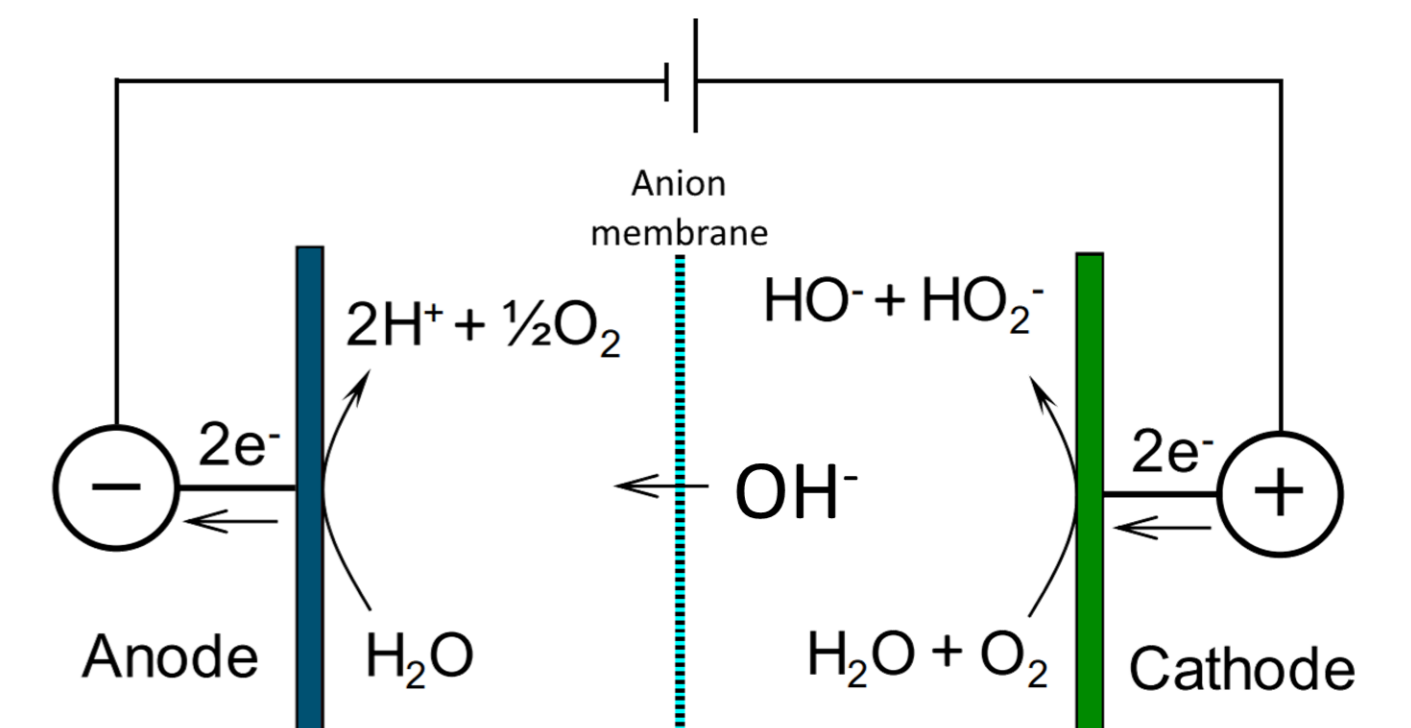
Objective

Investigation of particle size effect for Ni NPs for the production of hydrogen peroxide

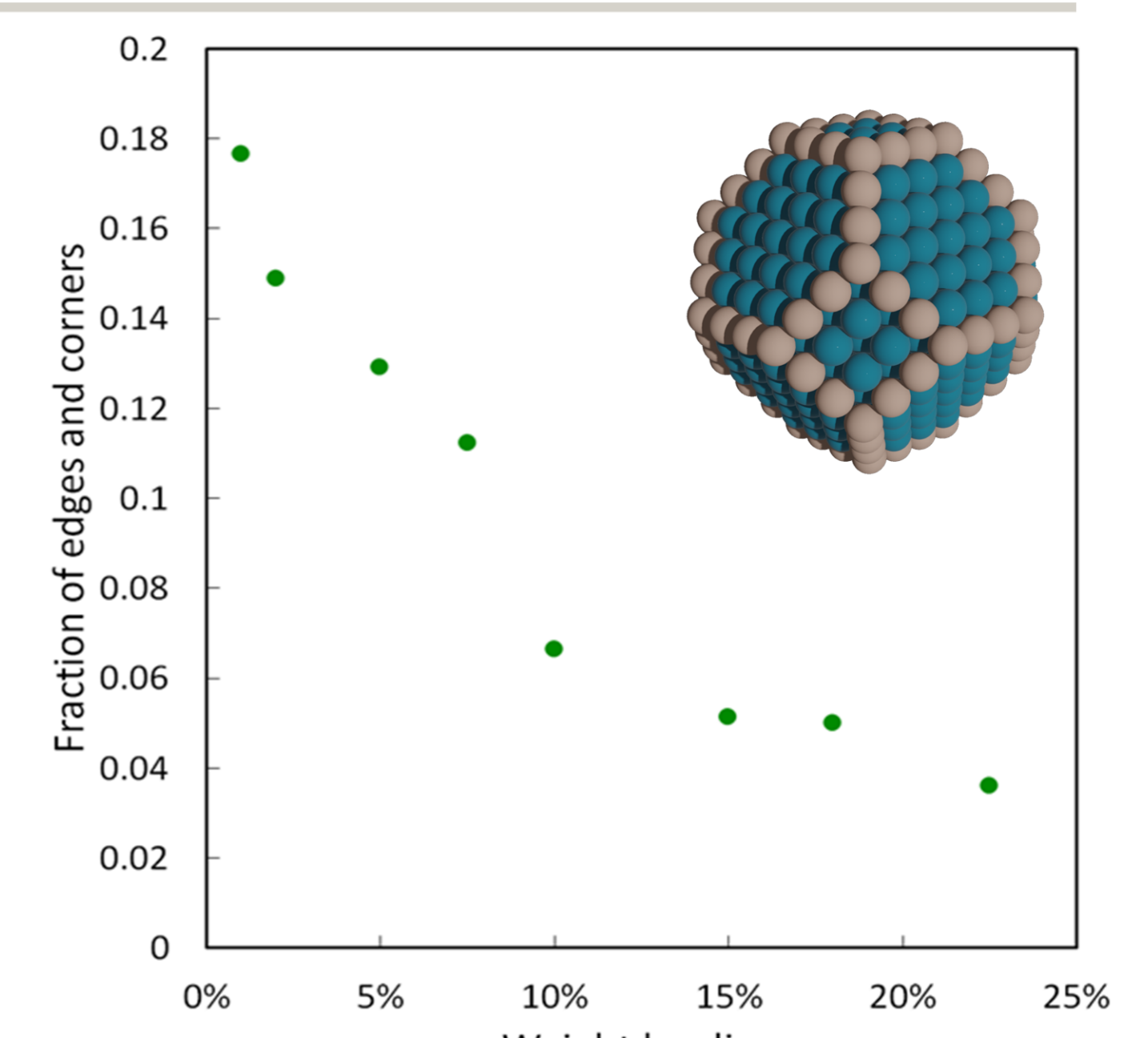
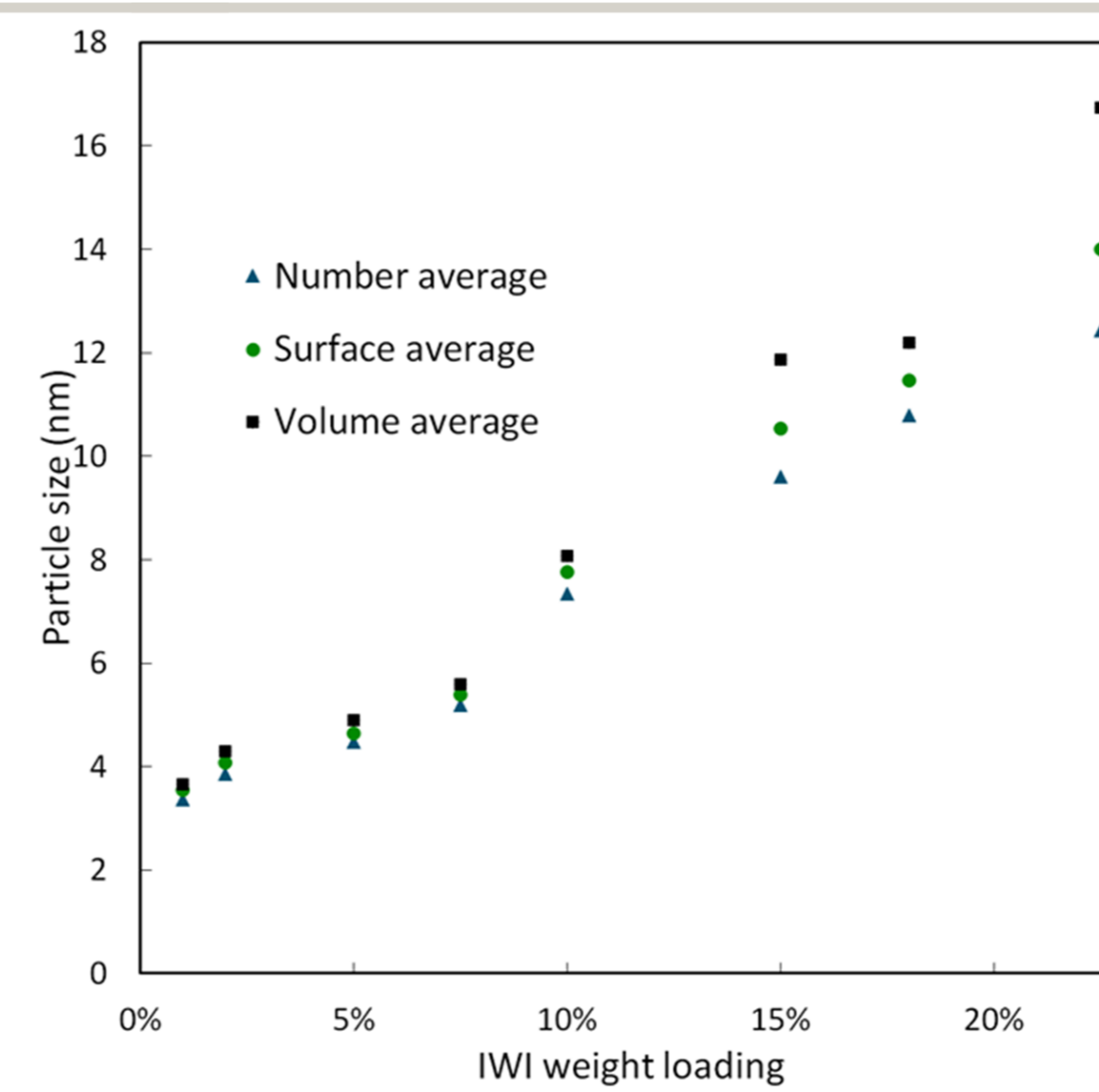
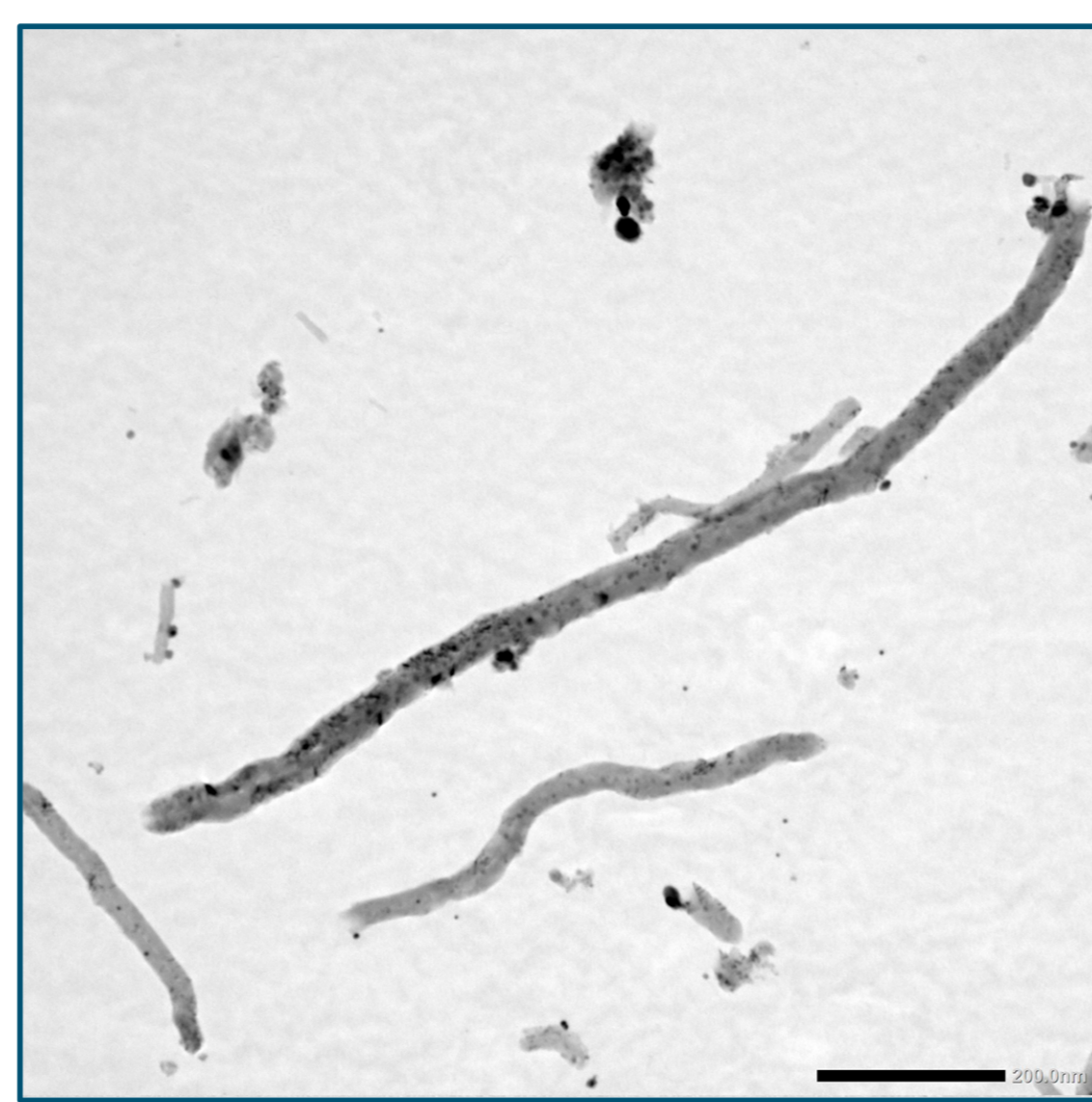
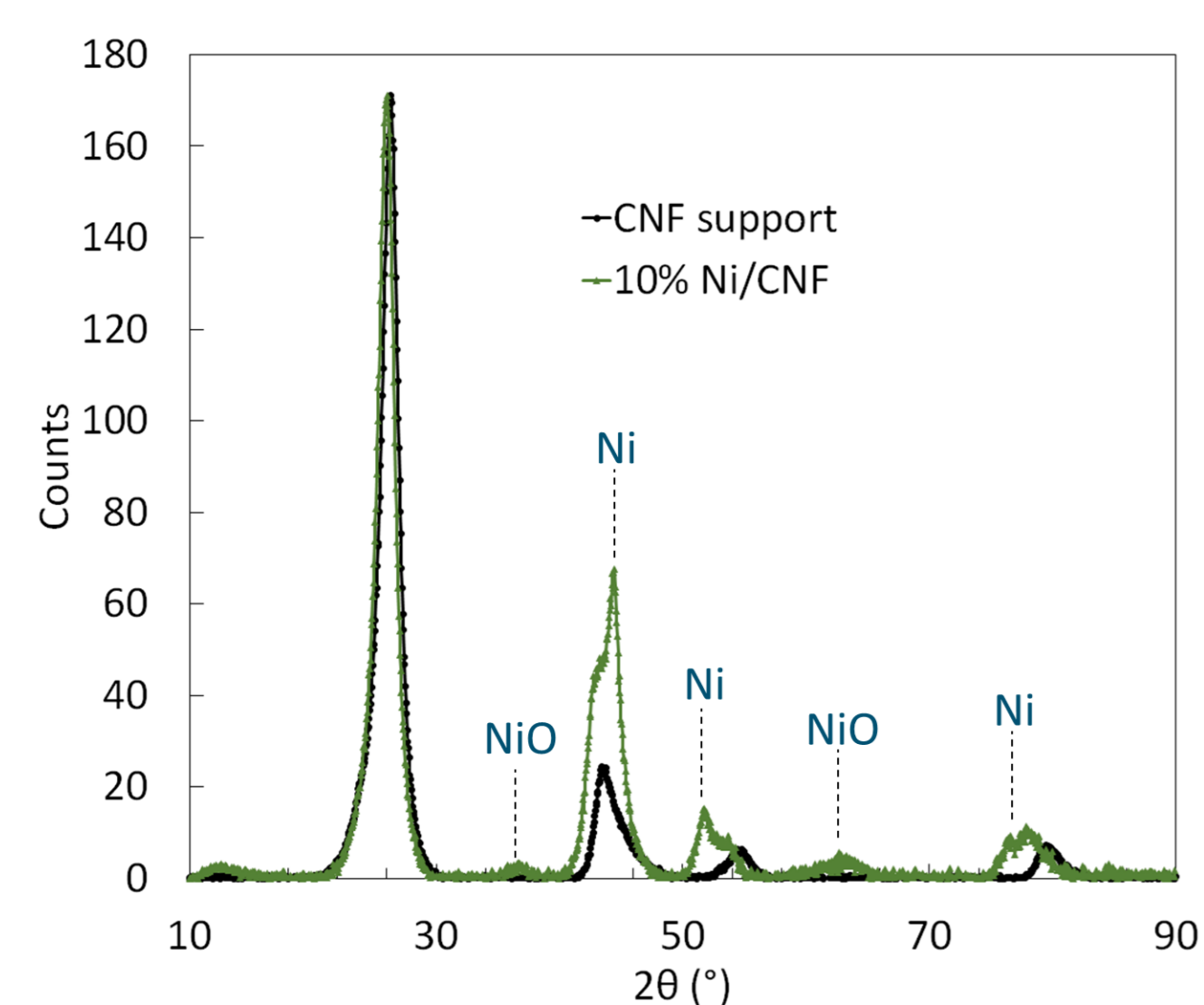


Approach

- Synthesize carbon nanofiber (CNF) support
- Create Ni NPs of different sizes with varying concentration of metal in impregnation solution
- Use geometric model to calculate edges and corners
- Determine property performance relationship



Characterization

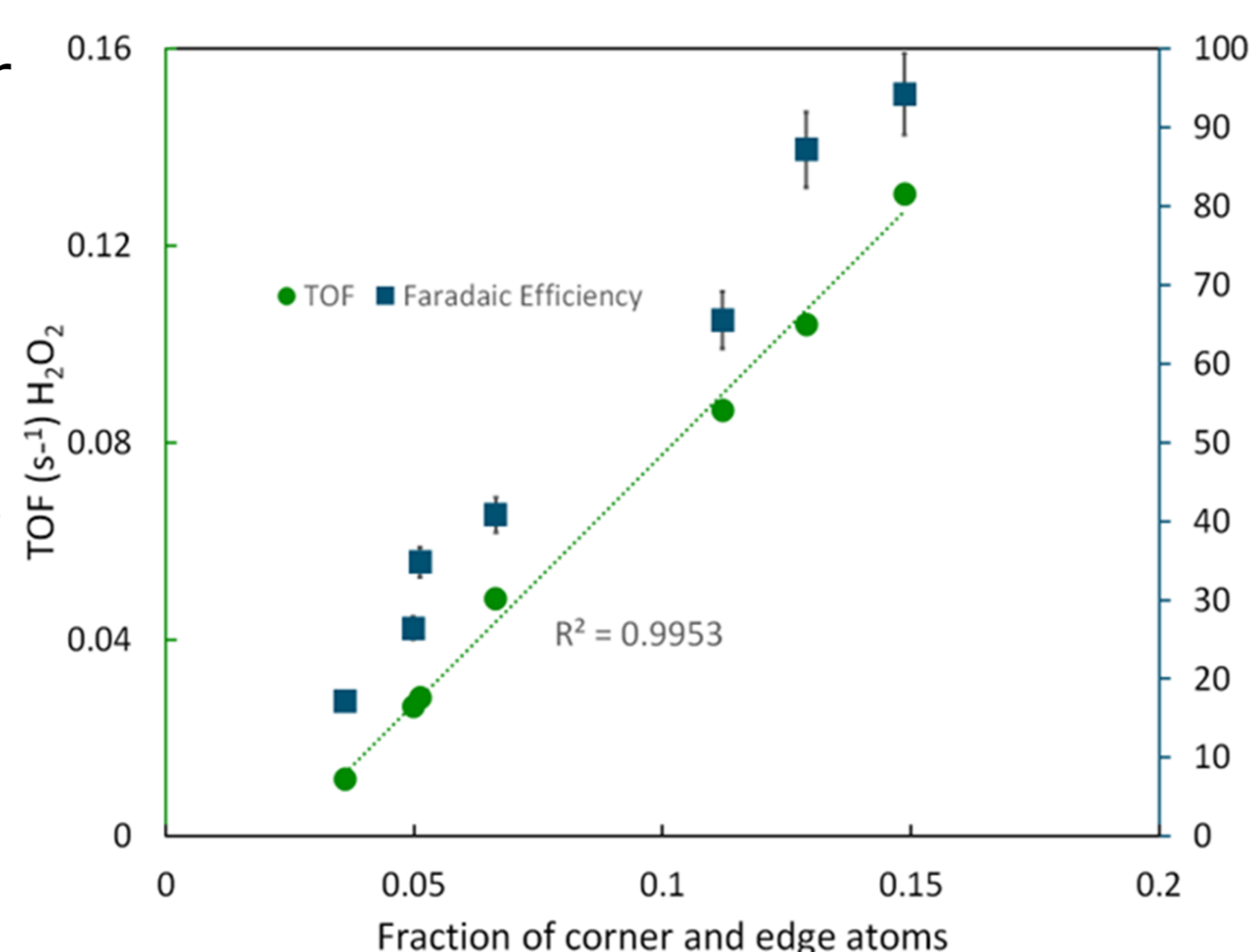


XRD and TEM analysis were used to determine particle size

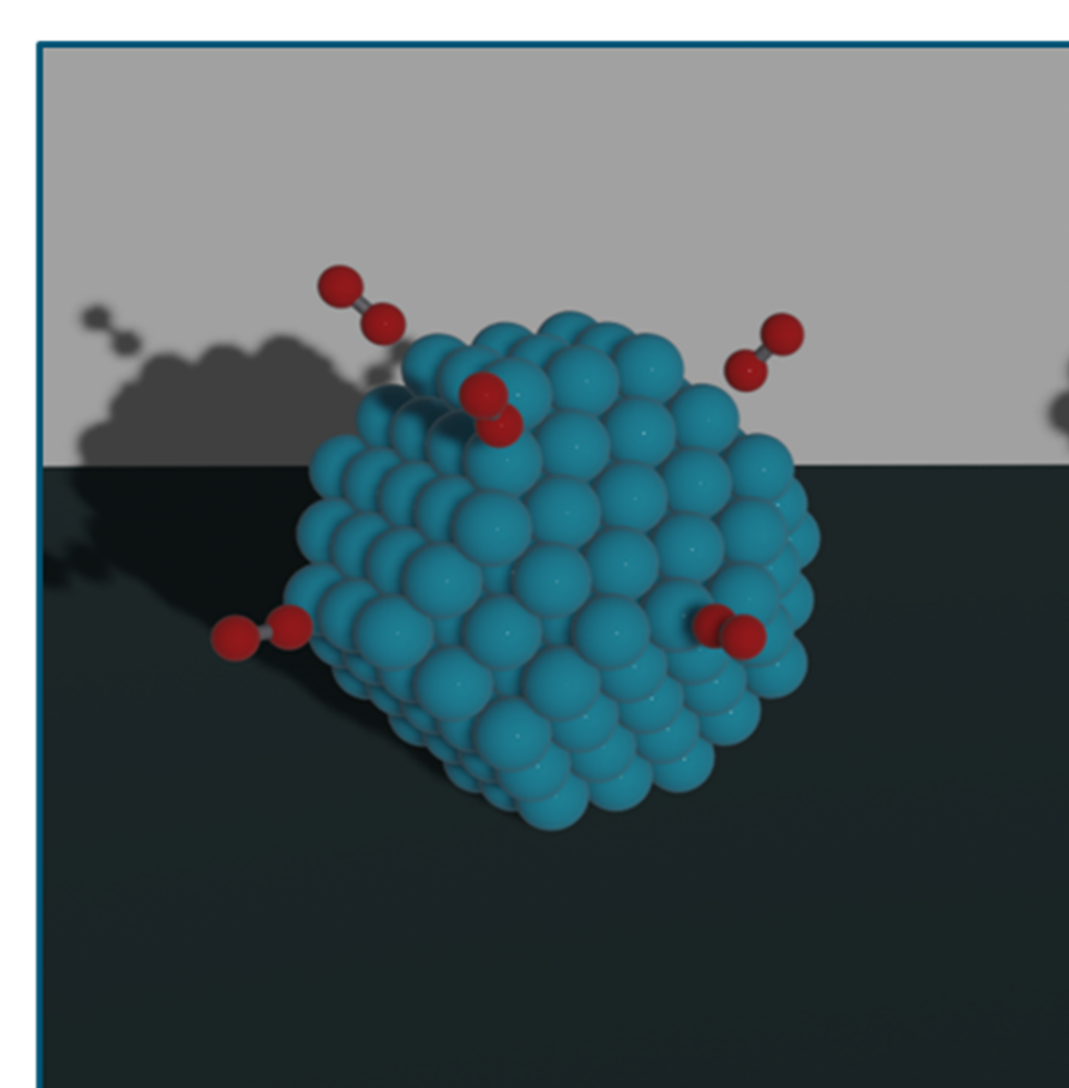
A geometrical model was used to determine amount of edge and corner atoms compared to facet atoms in nanoparticles

Catalytic performance

- Fraction of edges and corner vs. intrinsic activity (TOF)
- TOF increases with lower particle size
- Faradaic efficiency increases with lower particle size
- **Edges and corners are responsible for peroxide production**

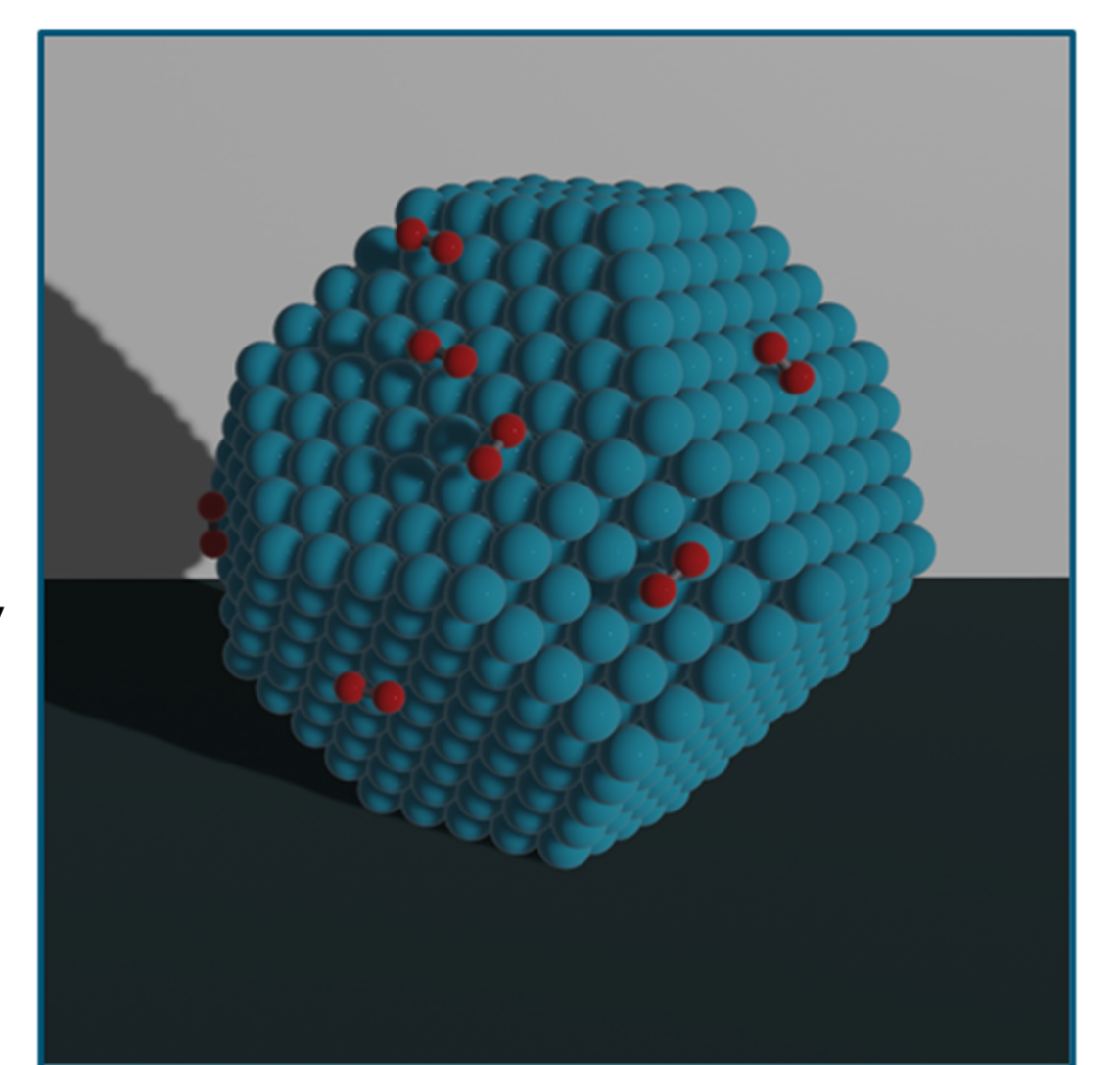


Influence of geometry



Smaller particles have more End-on ads at edges -> more H₂O₂

Lower fraction of edge and corner atoms
Lower efficiency



Larger particles have more Side-on ads at facets -> more side reactions

Conclusions

- The TOF and faradaic efficiency is strongly correlated with the amount of edges and corners of the nanoparticles
- Smaller particles are substantially more efficient for H₂O₂ production

Acknowledgements

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