Using Evolution to Discover Carbon Dioxide Reducing Catalysts

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Background

Emitted anthropogenic carbon dioxide (CO_2) must be minimised as it significantly contributes to the greenhouse effect. A partial solution to apply to industrial processes is to capture and convert discharged CO_2 to other products. Copper (Cu) surfaces have shown promise to selectively catalyse the reduction of CO_2 into hydrocarbons and alcohols; significantly more than other metals (example in Figure 1). However, the performance of the catalyst must still be increased to be viable for widespread use. A nanoparticle form of Cu offers such a pathway for catalytic improvement.

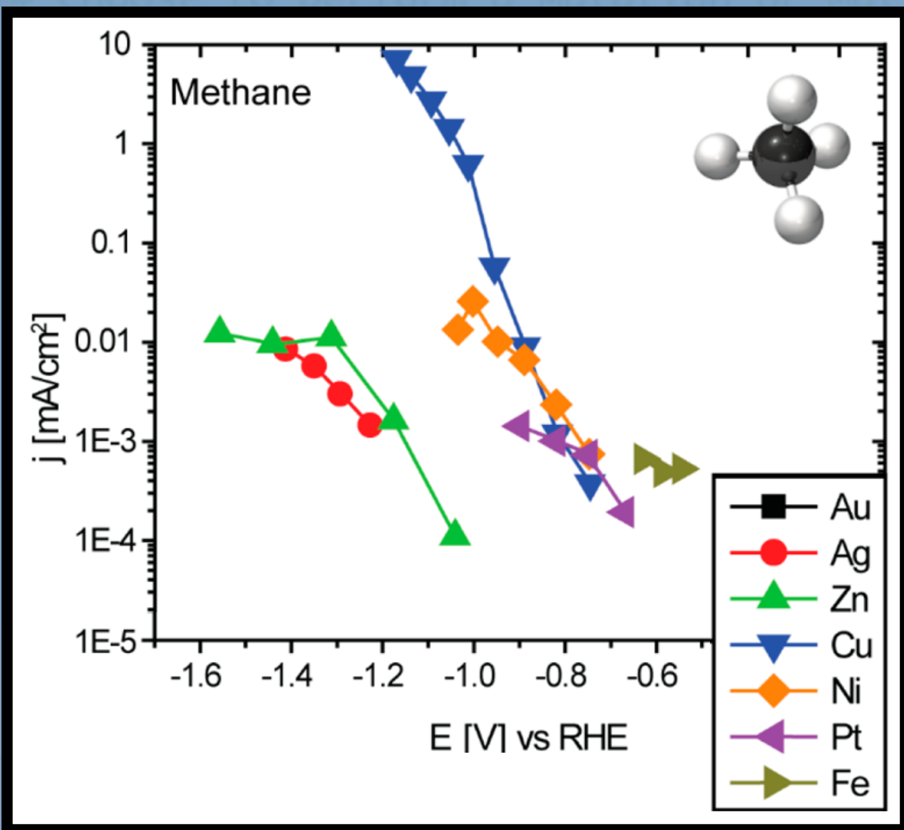


Figure 1: Current densities (j) for the reduction of CO_2 to methane for a variety of transition metal surfaces across different applied potentials (E).
K. P. Kuhl *et al.*, *J. Am. Chem. Soc.*, 2014, 136 (40), pp 14107–14113

Nanoparticles and their Structure

Nanoparticles have more rich surface features, such as corners, edges, and defects of these sites, compared to bulk surfaces (Figure 2). These can give nanoparticles interesting catalytic properties.

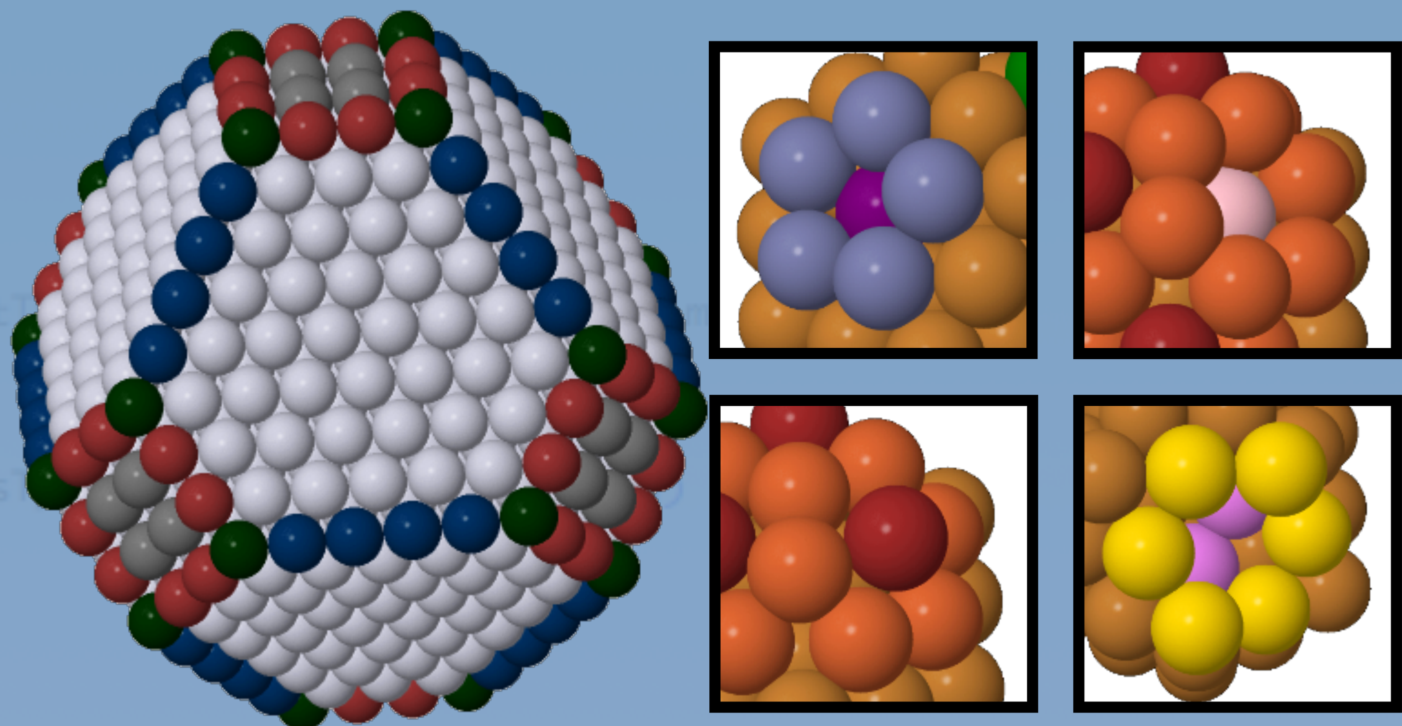
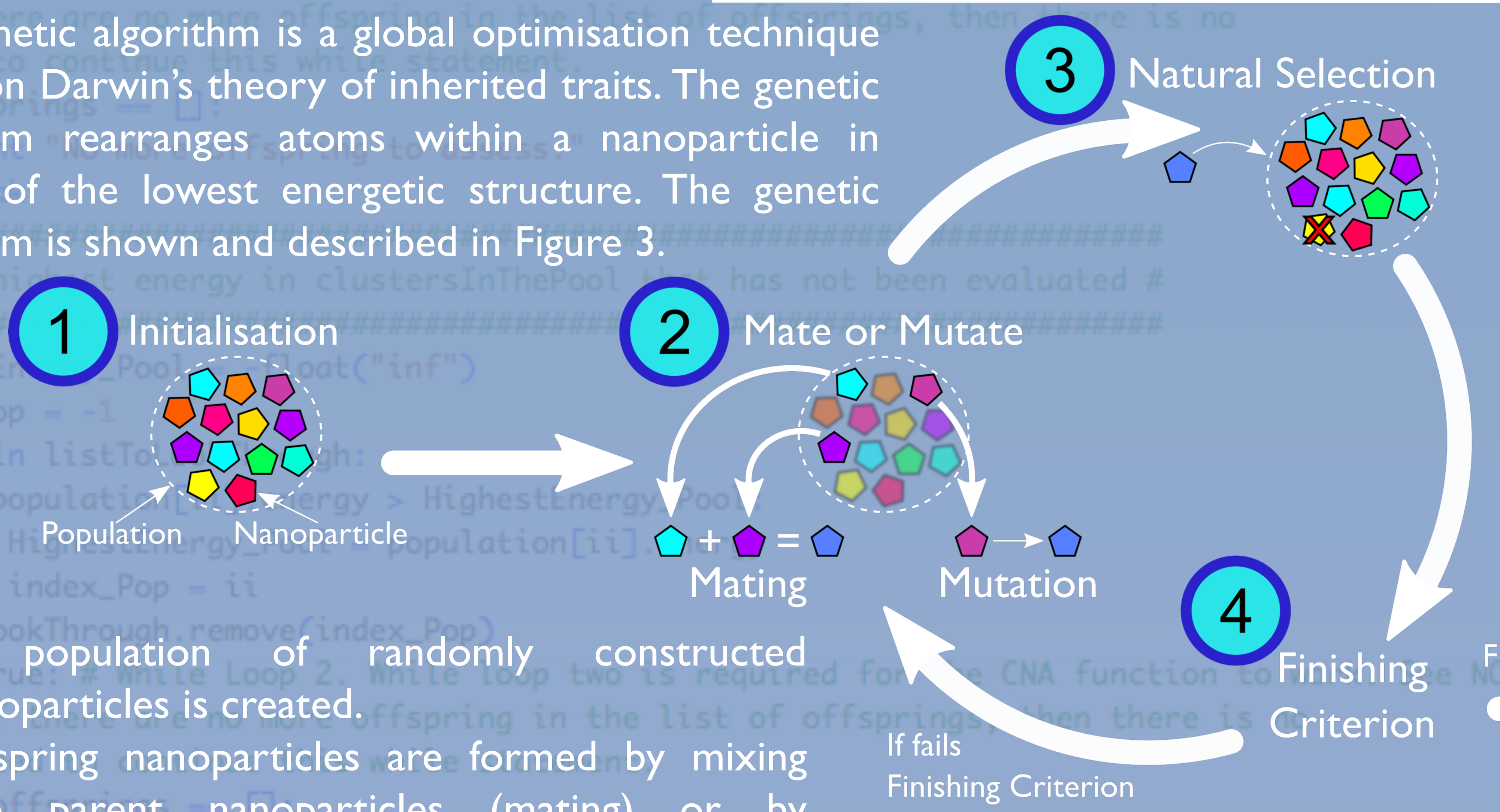


Figure 2: An example of a nanoparticle and various possible site defects. Corners and edges are coloured.

Before the catalytic properties of a nanoparticle can be explored, it is necessary to **obtain the stable structures of the nanoparticle** that would exist experimentally.

Method: The Genetic Algorithm

The genetic algorithm is a global optimisation technique based on Darwin's theory of inherited traits. The genetic algorithm rearranges atoms within a nanoparticle in search of the lowest energetic structure. The genetic algorithm is shown and described in Figure 3.



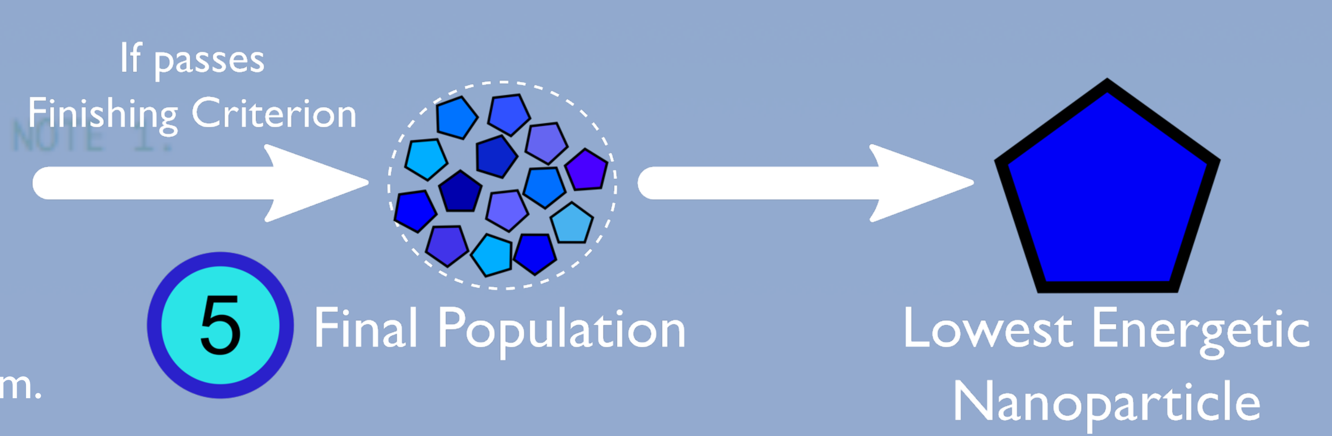


Figure 3: Diagram of the genetic algorithm.

1. A population of randomly constructed nanoparticles is created.
2. Offspring nanoparticles are formed by mixing two parent nanoparticles (mating) or by modifying an existing nanoparticle (mutation).
3. The fitness of both existing and offspring nanoparticles are assessed. Here, fitter nanoparticles are those with lower energies. Less fit individuals in the population are replaced by fitter offspring.
4. The population evolves through many generations by repeating steps 2 and 3 until a finishing criterion is met.
5. The genetic algorithm ends and the lowest energetic nanoparticle structure is obtained from the population.

Results and Future Directions

The lowest energetic structures of Cu_{55}, Cu_{78}, Cu_{101}, Cu_{124}, and Cu_{147} were obtained using the genetic algorithm (Figure 4). These structures contain interesting surfaces features, such as the twisted icosahedron structure exhibited by Cu_{78} and the intersection of the shell and the core seen in Cu_{101} (middle) and Cu_{124}, that could exhibit potential catalytic properties. Catalytic studies of these structures are currently being performed at the University of Iceland.

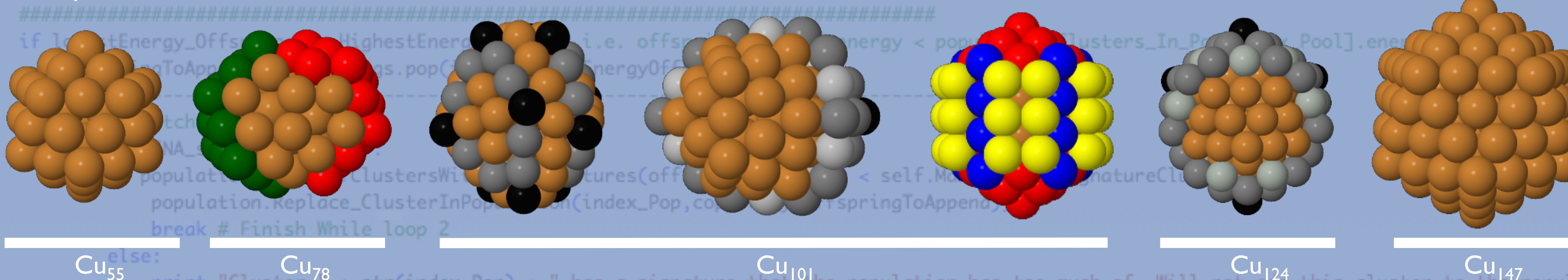


Figure 4: Lowest energetic structures of Cu_{55}, Cu_{78}, Cu_{101}, Cu_{124} and Cu_{147} nanoparticles.

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