

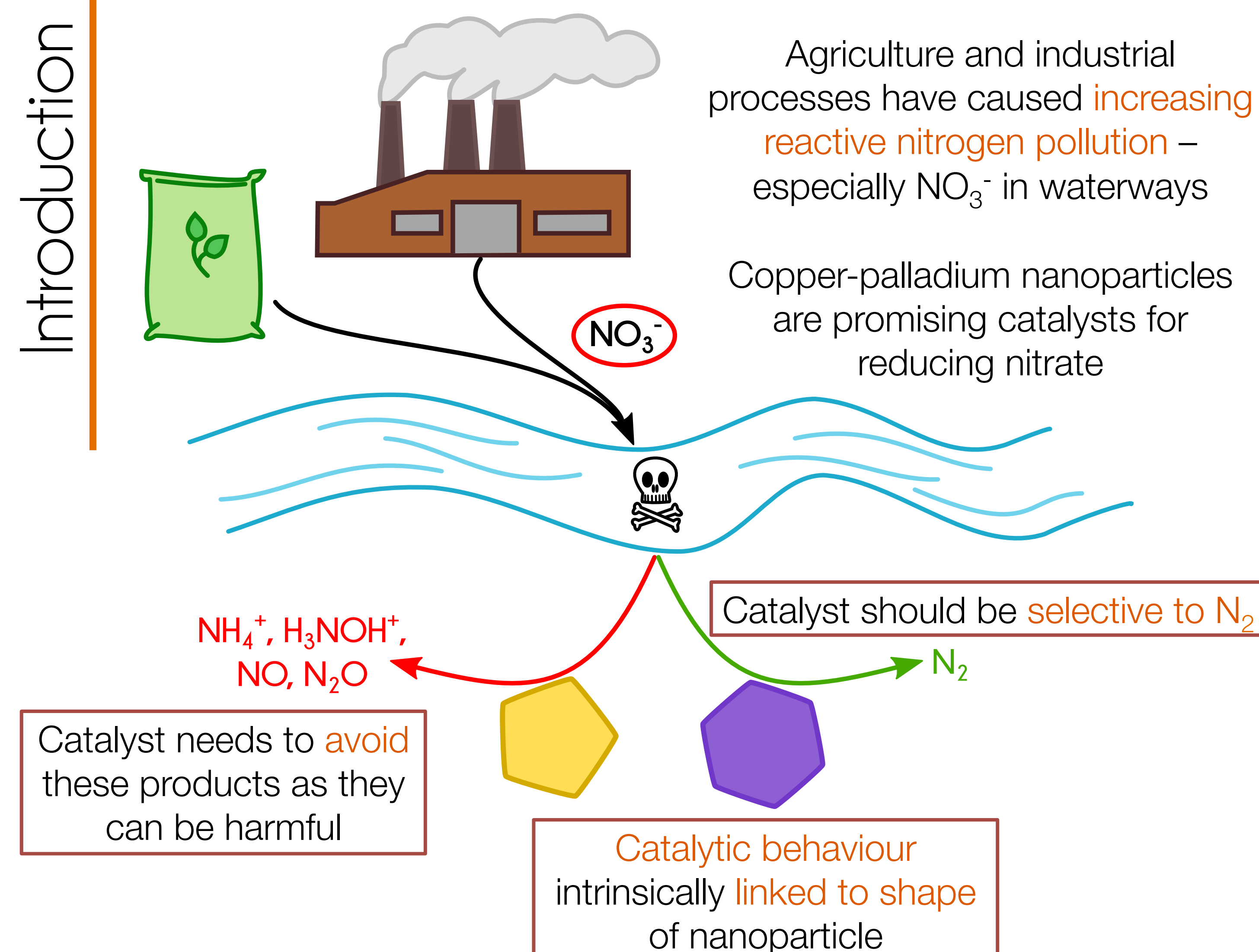
Nano-catalysts for Clean Water: The Structure and Segregation of CuPd Nanoparticles

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Introduction

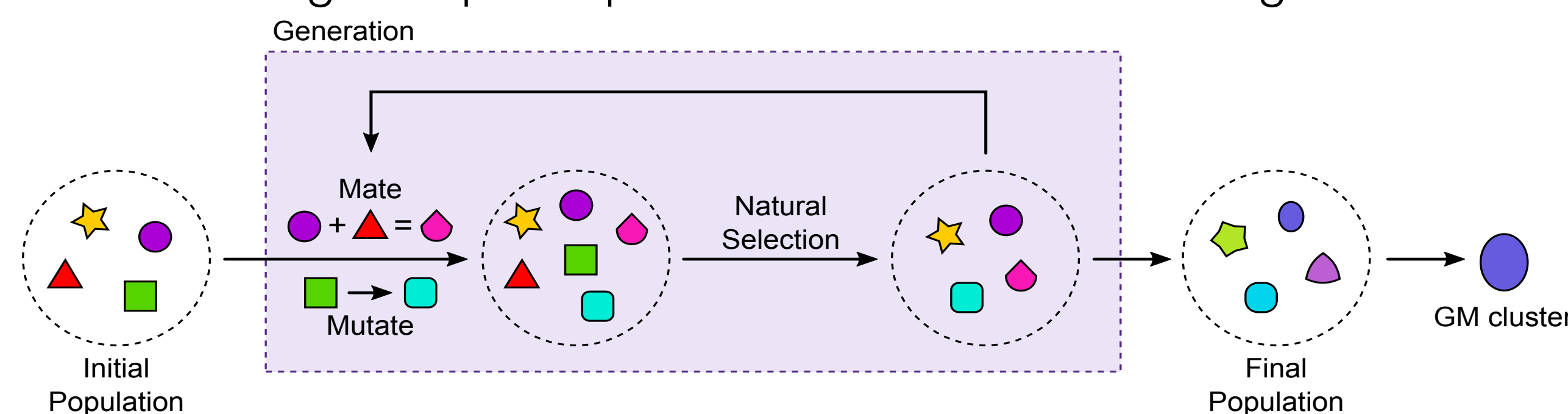


Selectivity to N_2 must improve before CuPd nano-catalysts are practically feasible.

Here, the structures of CuPd nanoparticles are investigated using computational methods.

Methods

Low energy nanoparticle structures were found using a genetic algorithm¹ using an empirical potential to describe the energetics

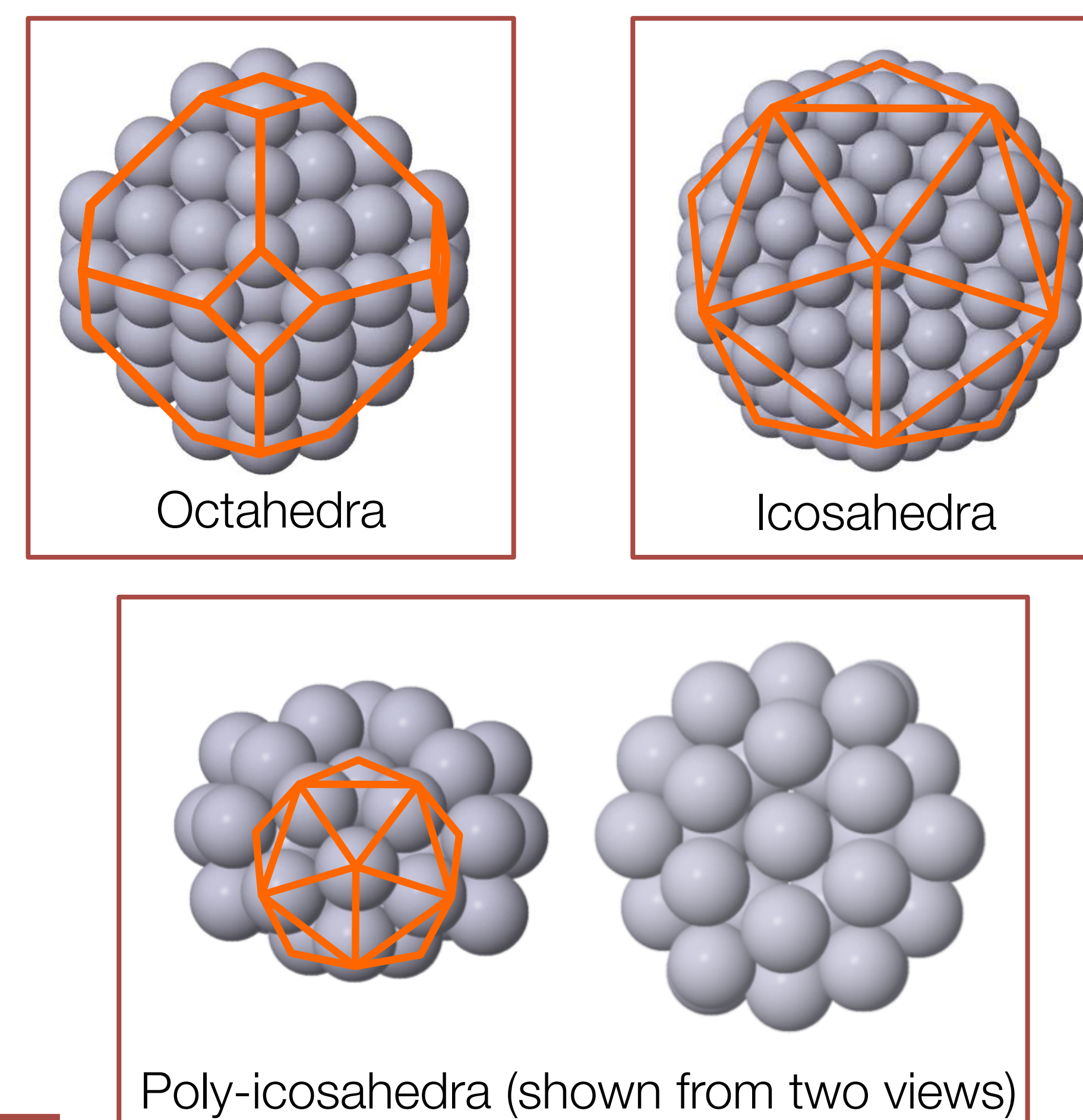


Nanoparticles further refined using density functional theory, using the PBE exchange-correlation functional, as implemented in VASP

¹ Weal, G. R.; McIntyre, S. M.; Garden, A. L. *J. Chem. Inf. Model* 2021, 61, 1732-1744

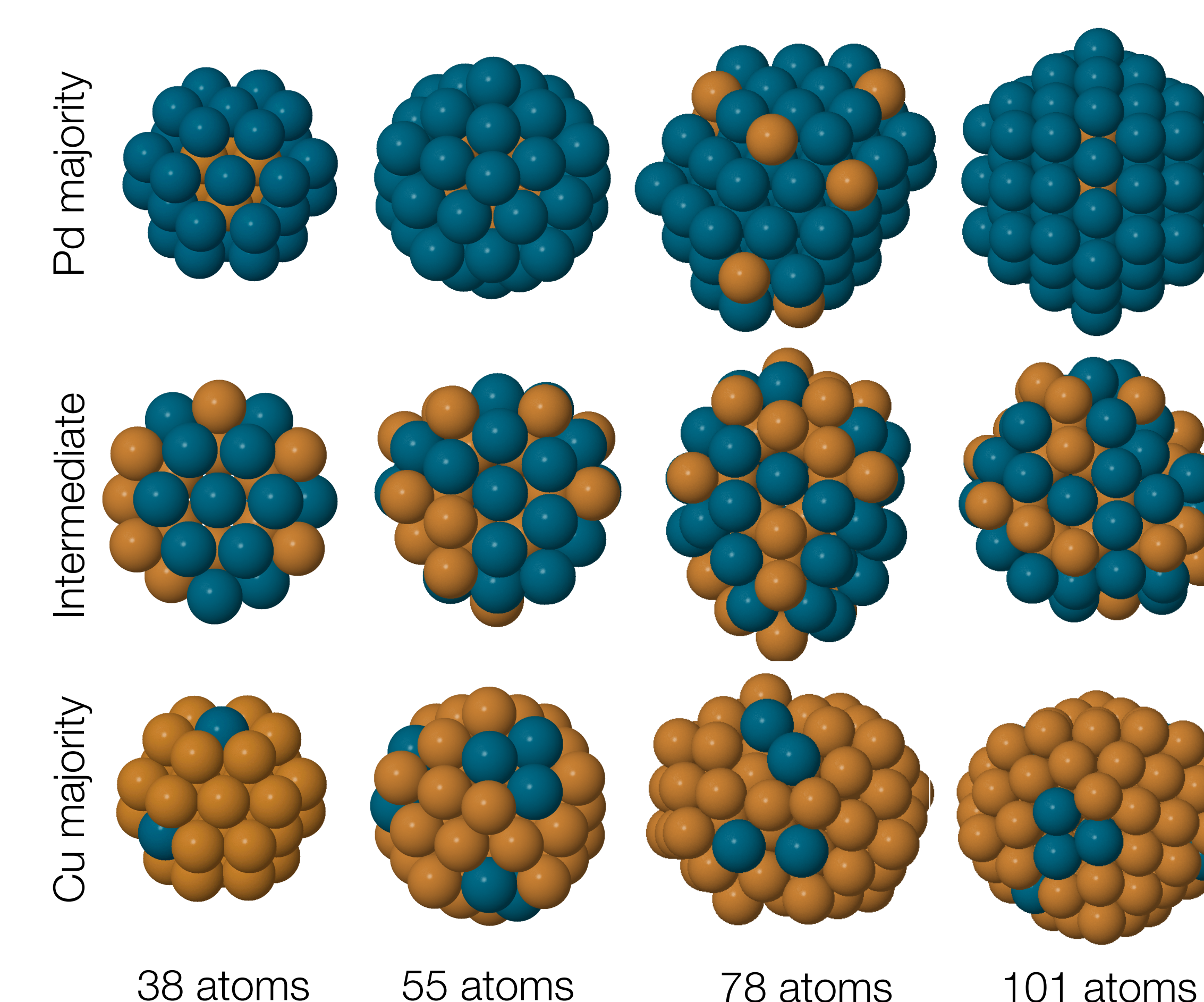
1 Nanoparticle Structure

Nanoparticle structures based on **three structural families** were predominant



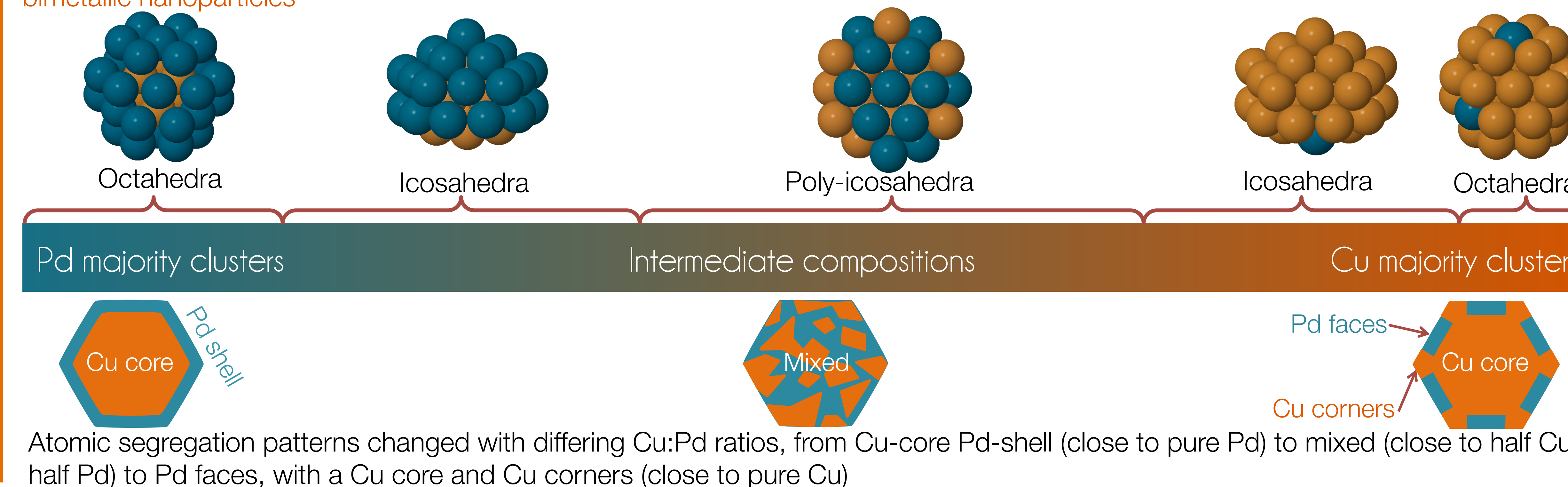
3 Impact of Size

Similar patterns in structure and segregation were seen across **four nanoparticle sizes**



2 Impact of Cu:Pd ratio

Structures were heavily **dependent on Cu:Pd ratio**. Ratios close to monometallic nanoparticles (pure Cu and pure Pd), octahedra are dominant. In intermediate regions (close to half Cu, half Pd) poly-icosahedra are dominant. Poly-icosahedra are **only seen for bimetallic nanoparticles**



Catalytic Implications

- Poly-icosahedra** are only seen for nanoparticles with both Cu and Pd atoms (and not the monometallic Cu or Pd nanoparticles) – they may be **crucial for CuPd nanoparticle catalysis**
- At most Cu:Pd ratios, **both Cu and Pd** atoms are present on the surface of the nanoparticles and thus **available for catalysis**
- Future computational studies should explicitly consider the NO_x reduction reaction on these nanoparticle structures



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