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Equitable Partitions in Inorganic Nanoclusters

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Introduction

We use **graph-theoretic** concepts with the twofold aim of

- offering a new description of **symmetry** in inorganic nanomaterials;
- correlating such a description with the **distribution of local properties**.

In particular, we demonstrate a link between the Equitable Partitions (EP) of chemical graphs [1-3] and the properties of the constituent atoms of inorganic nanoclusters.

Our method sheds new light on the structure-property relationships of inorganic nanomaterials. Our findings can have implications in the understanding, design, and engineering of magnetic nanoparticles, catalyst materials, and other applications at the nanoscale.

Materials and Methods

Systems: Spherical and polyhedral magnetic nanoclusters (e.g. α-iron, cobalt) extracted from bulk lattices of corresponding chemical elements.

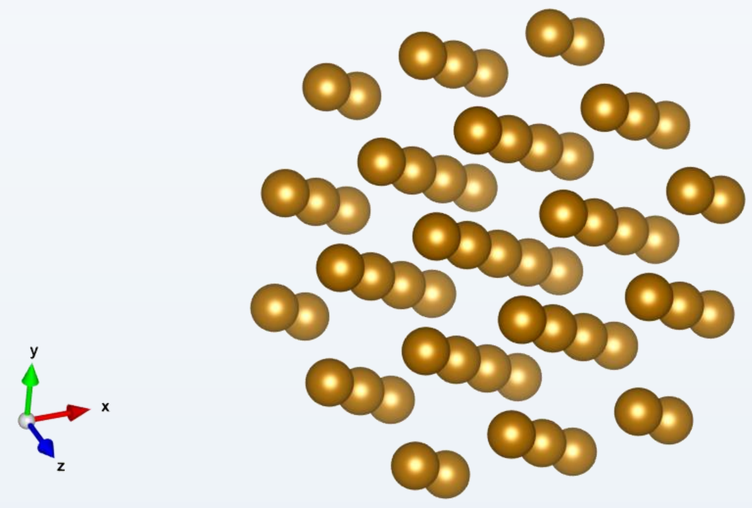
Graphs: Atom-atom edges defined by nearest neighbour adjacency (next-nearest neighbours were also considered for bcc iron).

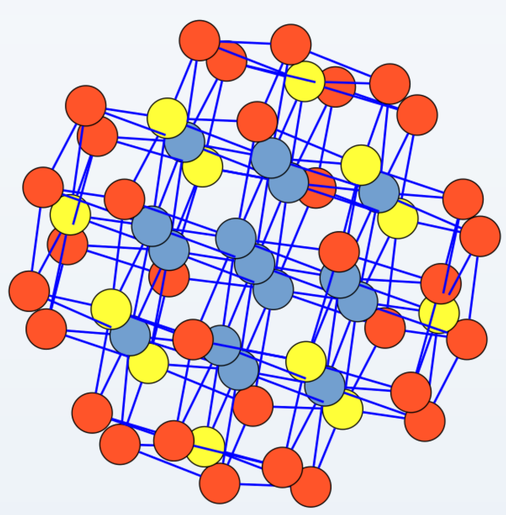
Equitable Partitions (EP): Classification of graph nodes (atoms) with uniform inter- and intra-class connectivity. We determined the coarsest EP.

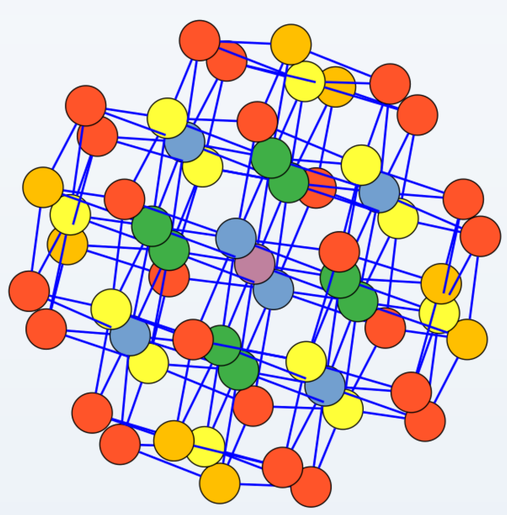
Local (Atom) **Properties**: Radial distance from particle centre; classical potential energy (e.g Lennard-Jones); measure of total force on atom; local charge density; local spin magnetic dipole moment. Last three are computed by **DFT** calculations using the **SIESTA** software package [4].

Results and Discussion

Values of all above computed local properties are invariably distributed according to the graph's **coarsest EP** (cEP); in other words, *all atoms in a given coarsest EP class, share the exact same properties*. Figures below illustrate typical examples.

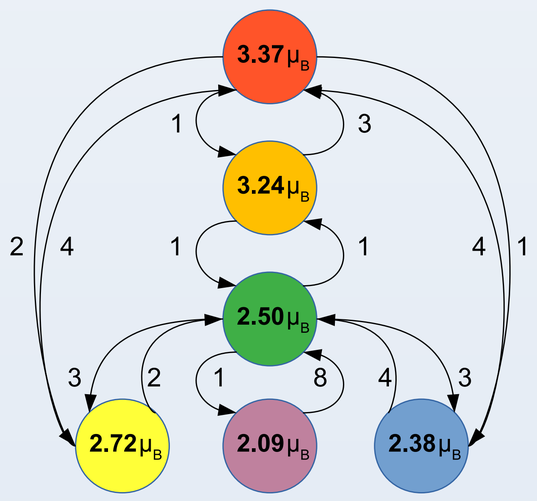






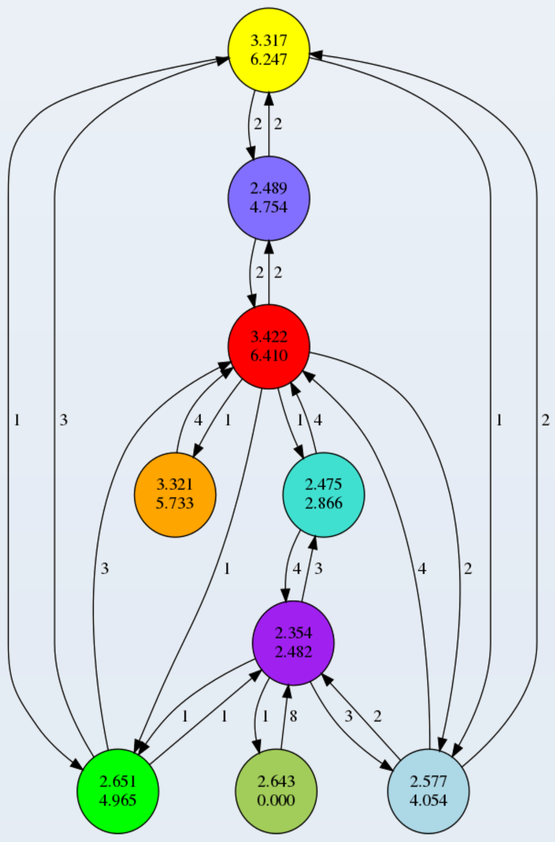
Example: 59-atom bcc-iron nanocluster

Magnetic nanoclusters subjected to spin-polarised calculations, exhibit local magnetic moments that vary with atom's position. While surface versus bulk effects are well known, the exact distribution of magnetic moments, is not fully understood.



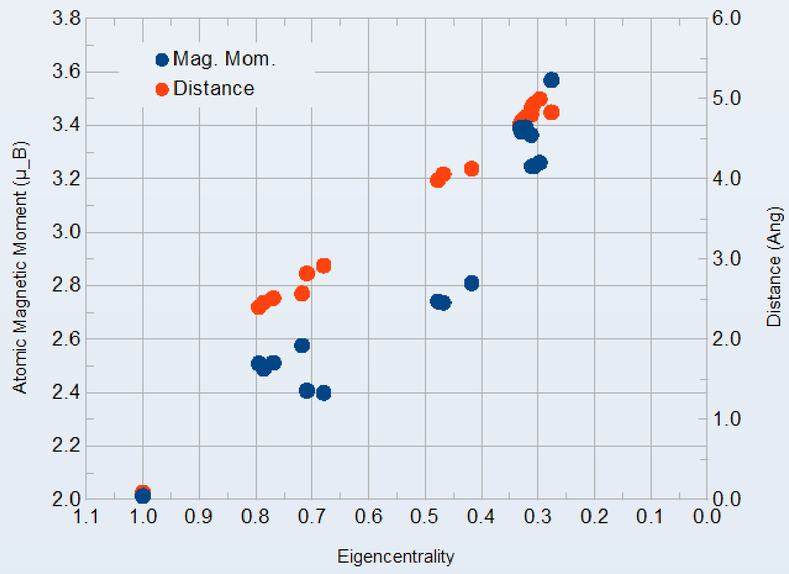
Same nanoparticle as a graph, *G*

Coordination numbers (red=4, yellow=6, blue=8) do play a role but are not the sole determinants of local magnetism. Atoms with same coordination numbers may differ in magnetic moments.



Coarsest Equitable Partition (cEP) of *G*

Equitable partitions classify atoms according to the equivalent places they hold in the graph, capturing the interactions with their environment.



Quotient graph (QG) according to the cEP of *G*

It is the directed graph defined when taking the cEP cells or classes as nodes. It describes pictorially the graph's coarsest EP. The partition of magnetic moments (values in circles) is also the coarsest equitable partition. **Right**: Quotient Graph of a 113-atom iron cluster. Values in circles are magnetic moments (top) and distances from cluster centre (bottom)

Equitable Partition and symmetry breaking

Defects (here: vacancy on the surface of 59-atom iron cluster) rearrange electron density and modify local magnetic moments. Their new distribution is captured by the new coarsest EP. Horizontal axis: Eigencentralities (principal eigenvector elements) also conform to the coarsest EP as per well known theorems.

Conclusions and Future Goals

- Nanocluster graphs are defined by means of *neighbour adjacency*.
- Thus, *spatial symmetries* are reflected in the *graphs' generalised symmetries*, as described by their *Equitable Partitions*.
- Therefore, *Equitable Partition classes* correspond to *identical spatial and interaction environments* of participant atoms.
- These, in turn, give rise to *identical values of local properties* when the latter depend on an atom's place in or interaction with its environment.
- Spin-orbit coupling and structural relaxation will be included in subsequent calculations, which will also cover Ni and alloy clusters.

References

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