Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

An Augmented (Multi-Descriptor) Grouping Algorithm to Optimize Chemical Ordering in Nanoalloys

Davide Fioravanti[1], Giovanni Barcaro[1*], Alessandro Fortunelli[2*]

[1]CNR-IPCF, CNR Research Area, Via Moruzzi 1, 56124 Pisa

[2]CNR-ICCOM, CNR Research Area, Via Moruzzi 1, 56124 Pisa

Corresponding authors: alessandro.fortunelli@cnr.it, giovanni.barcaro@cnr.it

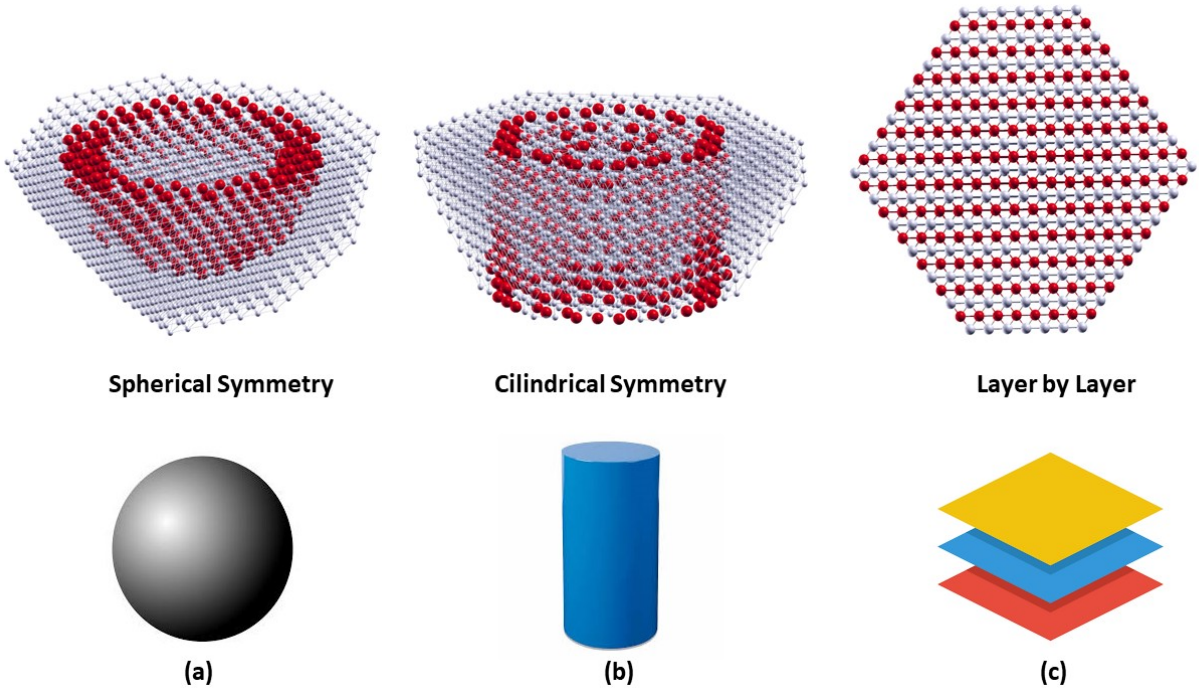

Figure S1: (a) spherical, (b) cylindrical and (c) layer-by-layer grouping schemes realized in a Truncated Octahedron (TO) made of 4033 atoms. In (a) and (b) half of the TO structure is visualized for better clarity. These are schematic representations of possible ways of breaking the symmetry of the system represented in the (a) scheme.