NANOCLUSTERS AND NEW MATERIALS: PROBING THE LOW ENERGY LANDSCAPE OF NANOSCALE SILICA

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The fabrication and study of silica (SiO_2) nanostructures has received considerable attention in recent years, largely due to their potential in applications as diverse as photonics/optics, microelectronics, bionanotechnology and catalysis. SiO_2 is particularly interesting as a nanoscale oxide building material due to its stability and the ease with which its inherent structural richness can be exploited via a range of synthetic methods. Via extensive global optimisations, employing interaction potentials specifically parameterised for nanoscale silica, and subsequent ab initio refinement, we accurately characterise the low energy potential energy landscape of silica nanoclusters for $(SiO_2)_N$ 2-30. Nanostructures in general, are known to possess characteristic motifs, not present in their bulk analogues, giving rise to novel size-dependent properties. Our SiO_2 clusters are truly of the nanoscale, possessing dimensions of up to 3 nm, and are found to display remarkable structural forms not exhibited in any known bulk silica polymorph. Our results reveal a wealth of size dependent properties for nano-SiO_2 including: (i) the occurrence of especially stable “magic” clusters [1,2], (ii) regular electronic and morphological fluctuations depending on the number of SiO_2 units [2], (iii) a 1D to 2D transition from columnar cluster topologies to disklike clusters [2], (iv) the emergence for larger clusters of energetically favourable surface reconstruction via Si_2O_2-rings giving rise to low energy fully-coordinated clusters [2-4] – in line with recent SiO_2 thin film studies [5,6]. Considering the morphologies and stabilities of the discovered silica nanostructures new materials are proposed employing $(SiO_2)_N$ clusters as nanoscale building blocks. The novel properties of such silica nanocluster-based materials are also discussed.

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