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Structure Prediction of Manganese Dioxide Nanoclusters Using Computer Simulation Techniques

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Abstract content
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The characteristics of nanoclusters are linked to the high value of their surface/volume ratio, and therefore the structure of nanoclusters plays an important role in determining their physical properties. Manganese dioxide as a well-known transition-metal oxide is one of the most attractive inorganic materials because of its structural flexibility and wide range applications in many chemical processes such as ion exchange, separation, catalysis, molecular adsorption, biosensors and energy storage in batteries and supercapacitors. In order to enhance the properties of MnO₂ for various applications, some new or modified MnO₂ compounds are developed recently. One of the major demands for developing these materials is to modify and strengthen the structural stability in order to prevent the rapid capacity fading during the process of charge/discharge cycling. The interest in synthesis and characterisation of nanoclusters is driven by a wide range of applications of nanoparticle materials in catalysis, electronics and energy conversion. The lowest energy configurations for (MnO₂)_n clusters, n =1 to 10 are predicted, employing the interatomic potential technique and electronic structure density functional theory method at the PBEso10 level. The application of an evolutionary algorithm to different energy landscapes, as defined by interatomic potentials, for each cluster size was used to generate the plausible structures for refinement using DFT. The order of stability and degeneracy of different sizes of nanoclusters are investigated. In addition, geometric properties of the nanoclusters are predicted. The DFT based, MnO₂ global minima nanoclusters were found to be similar to those predicted for isostructural TiO₂.

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