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Structure Prediction of $(\text{BaO})_n$ nanoclusters for $n \leq 24$ using an evolutionary algorithm

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Abstract

Knowing the structure of nanoclusters is relevant to gaining insight into their properties for materials design. Computational studies predicting their structure should aim to reproduce experimental results. Here, barium oxide was chosen for its suitability for both computational structure prediction and experimental structure determination. An evolutionary algorithm implemented within the KLMC structure prediction package was employed to find the thermodynamically most stable structures of barium oxide nanoclusters $(\text{BaO})_n$ with $n = 4$ to 18 and 24. Evolutionary algorithm runs were performed to locate local minima on the potential energy landscape defined using interatomic potentials, the structures of which were then refined using density functional theory. BaO clusters show greater preference than MgO for adopting cuts from its bulk phase, thus more closely resemble clusters of KF. $(\text{BaO})_4$, $(\text{BaO})_6$, $(\text{BaO})_8$, $(\text{BaO})_{10}$ and $(\text{BaO})_{16}$ should be magic number clusters and each are at least 0.03 eV/BaO more stable than all other PBEsol local minima clusters found for the same size.

Keywords: inorganic nanoclusters, global optimization, evolutionary algorithm, computational modelling, barium oxide

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