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Prediction of Structures and Energy stabilities of VO₂ nanoparticles.

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Abstract content
   (Max 300 words)
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We have employed a Genetic Algorithm (GA) Hybrid technique as implemented in GULP code to predict the ground-state energies of various small V_nO_{2n} nanoparticles (n = 1-15). The search procedures were based on the GA techniques and the Interatomic Potential (IP) model, and did not refer to any known VO₂ polymorphs. All stable structures were optimized using Density Functional Theory (DFT) employing Dmol code. More importantly, ground state VO₂ nanoparticles (clusters n = 1-3), were identified. The results showed that for n = 1 (VO₂), the energies of both the core and shell candidate structures were found to be similar. As n increases, the symmetry changed from D2h to C2v and the structures became more stable. Interestingly, their atomic arrangements were also observed to be similar to those of TiO₂. Furthermore, the O-V-O bond angles for both the core and shell models (111.2o) compare well with those for titania (111.4o).

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