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Title: Cluster Structure Selection Based on Highest Electron Affinity: The Case of TiO₂ Clusters

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TiO₂ clusters have attracted much attention owing to their potential applications in photovoltaics, photochemistry, and catalysis. We study the structure and electronic properties of (TiO₂)₂₋₁₀ clusters using basin hopping based on density functional theory, combined with many-body perturbation theory in the G₀W₀ approximation. We show that in photoemission experiments performed on anions the isomers with the highest electron affinity are selectively observed rather than those with the lowest energy. These isomers possess a highly reactive Ti³⁺ site. The selectivity for highly reactive clusters may be exploited for applications in photochemistry and catalysis.