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Nanocrystals

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Formation, Stability, and Chemistry of Tetravalent Actinide Nanocrystals

PI: Ping Yang, T-1

First database with almost 4000 stable structures for thorium dioxide (ThO_2)_n ($n \leq 8$) calculated with density functional theory.

The figure shows the lowest energy minima for different units of ThO_2 and the energy landscape generated by the found stable structures for Th_8O_{16} . This highlights the structural richness of the Th-O interactions.

