Abstract Submitted
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New Crystal Structures Identified for PtO and PtO_2 using Density Functional Theory Calculations[1] JUAREZ L.F. DA SILVA, RICARDO K. NOMIYAMA, University of Sao Paulo, MAURICIO J. PIOTROWSKI, Federal University of Santa Maria — Platinum plays an important role in catalysis and electrochemistry, and it has been known that the direct interaction of oxygen with Pt surfaces can lead to the formation of platinum oxides (PtO_x), which can affects the reactivity. To contribute to the atomistic understanding of the atomic structure of PtO_x, we report a density functional theory study of the atomic structure of bulk PtO_x ($1 \leq x \leq 2$). From our calculations, we identified a lowest energy structure (GeS-type, space group *Pnma*) for PtO, which is 0.181 eV lower in energy than the structure suggested by Moore and Pauling (PtS-type). Furthermore, two atomic structures were identified for PtO_2, which are almost degenerate in energy with the lowest energy structure reported so far for PtO_2 ($CaCl_2$-type). Based on our results and analysis, we suggest that Pt and O atoms tends to form octahedron motifs in PtO_x even at lower O composition by the formation of Pt−Pt bonds.

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