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Computational study of the pressure behavior of post-perovskite phases RAZVAN CARACAS, Geophysical Laboratory, Carnegie Institution of Washington, RONALD COHEN, Geophysical Laboratory, Carnegie Institution of Washington — The recent discovery of the post-perovskite phase transition ($CaIrO_3$ structure) in $MgSiO_3$ has lead to theoretical and experimental investigations of silicates, germanates and oxides that could take this structure. We have employed density functional-theory to explore a series of new compounds with the post-perovskite structure under pressure. We analyze the effects of the Si substitution by tetravalent cations on the perovskite-to-post-perovskite transition and on the crystal structure of post-perovskite. Cations Ti^{4+} and Zr^{4+} prefer the post-perovskite structure. We also explore the sesquioxides Al_2O_3 and Rh_2O_3 and compare their structural evolution with the one of $MgSiO_3$. For Rh_2O_3 we observe an enhancement of the ionic character of the type II structure with pressure.

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