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Prediction of an ultrahigh-pressure form of Al_2O_3[1] KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science, University of Minnesota — We predict by first principles a pressure induced phase transition in alumina at ∼3.7 Mbar, relevant for interiors of the giant planets and terrestrial exoplanets, at room temperature from the $CaIrO_3$-type polymorph to another with the U_2S_3-type structure. This transformation should be important for the analysis of shock data in this pressure range, since alumina is used as window material. Our calculated compression curves agree with shock data excellently, indicating that the presence of two phase transitions (corundum–Rh_2O_3(II)-type and Rh_2O_3(II)-type–$CaIrO_3$-type) had gone unnoticed in shock data. Our prediction suggests that the multi-Mbar crystal chemistry of planet-forming minerals might be related to that of the rare-earth sulfides.

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