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The high-pressure structural phase transition in heavier RH3 (R: rare earth metals) by ab initio theory WEI LUO, RAJEEV AHUJA, Condensed Matter Theory Group, Department of Physics, Uppsala University, Box 530, S-751 21, Uppsala, Sweden — Rare earth hydrides are very interesting because they exhibit a reversible metal-insulator transition upon hydrogenation. In present work, we have studied the structural stabilities of heaver rare earth trihydrides, RH3 (R=Sm, ..., Lu), under high pressure using ab initio calculations. Our results show the hexagonal structure with HoD3-type structure is stable for all studied RH3 at ambient pressure. Further these RH3 transform to a face-center cubic structure under high pressure. In HoD3-type phase bulk modulus decreases, whereas the transition pressure for hexagonal to fcc structural transformation increases, as the atomic number of rare earth element increases.

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