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Computational studies of layered trititanates with magnetic doping[1] CALEB HEATH, SALVADOR BARRAZA-LOPEZ, Z RYAN TIAN, Univ of Arkansas-Fayetteville — Layered titanate nanostructures are of great interest due to their ease of synthesis, modifiability, and variety in application. A profusion of experimental literature exists for these compounds but existing computational work has been limited in both quantity and scope. We examine hydrogen trititanate ($H_2Ti_3O_7$) with and without magnetic substitutional doping. Band structure, elastic properties, material stability, and magnetic properties of these titanates will be discussed.

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