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Equilibrium magnetic structure of NpSn_3 M. TAGHI FALLAHI, ZAHRA NOURBAKHSI, University of Isfahan, UNIVERSITY OF ISFAHAN TEAM — Actinide based compounds show very interesting physical properties due to the singular behaviour of their 5f electrons. The variation of these properties yields information on the electronic structure of the solid. We have focused on the NpSn_3 which exhibits antiferromagnetic phase at zero pressure. In this work to investigate the magnetic properties of NpSn_3 , the total energy per primitive unit cell as a function of its volume in antiferromagnetic, ferromagnetic and nonmagnetic phases are calculated using density functional theory within GGA and LDA approaches. We have found an antiferromagnetic ground state for NpSn_3 in both approaches. We have also found that for unit cell volumes smaller than a certain value, the magnetic moment is quenched and therefore the two antiferromagnetic and nonmagnetic curves coincide. For larger volumes a net magnetic moment appears and the antiferromagnetic curve branches off the nonmagnetic one. The branching volumes found in different approaches are different.

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