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On the stability of perovskite and post-perovskite polymorphs of $MgSiO_3$ JOSE MARTINS, INESC-MN, Rua Alves Redol 9, 1000-029 Lisboa, Portugal, YAOWEN LIU, INESC-MN, Rua Alves Redol 9, 1000-029 Lisboa, Portugal, *Present address: Department of Physics, Tongji Univ., Shanghai ,Chaina, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis MN 55455 — The relative stability of 10 distorted perovskite structures of $MgSiO_3$ have been investigated by first principles and contrasted with that of the newly found *Cmcm* post- perovskite. The electronic structure of these polymorphs was analyzed and simple relationships between magnitudes of polyhedral distortions, bond-lengths, and band-gaps were found. Up to approximately 95 GPa, the *Pnma* phase is the most stable, has the largest band gap, and can accommodate the largest volume reduction with the smallest distortion of the SiO_6 octahedra. At higher pressures the post-perovskite polymorph is the most stable one. This phase transition is accompanied by an increase of octahedral volume and band gap. These results do not support a transition from *Pnma* to another distorted perovskite structure prior to the transition to the *Cmcm* polymorph as proposed by some experiments.

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