Abstract Submitted for the MAR12 Meeting of The American Physical Society

Fate of MgSiO3 post-perovskite at multi-Mbar pressures¹ KOICHIRO UMEMOTO, University of Minnesota, SHUNQING WU, Iowa State University and Xiamen University, China, MIN JI, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University, RENATA WENTZCOVITCH, University of Minnesota — The discovery of the post-perovskite (PPV) transition of MgSiO₃ in 2004 invited a new question: What would be the next phase transition from the PPV phase? The importance of this question has increased, since many terrestrial exoplanets with masses of a few to 10 times Earth's (super-Earth) have been recently discovered. Here we predict the new class of phase transitions of MgSiO₃ PPV under ultrahigh pressure by first-principles calculations combined with the adaptive genetic algorithm, which is a powerful tool for blind structural searches for systems with the large number of atoms. We discuss implications of these new phase transitions in modeling of interiors of terrestrial exoplanets.

¹KU, SQW, JM, CZW, and KMH was supported by the US Department of Energy, Basic Energy Sciences, Division of Materials Science and Engineering, under Contract No. DE-AC02-07CH11358/ KU and RMW was supported by NSF grants ATM-0426757 (VLab) and EAR-1047629.

Koichiro Umemoto University of Minnesota

Date submitted: 11 Nov 2011 Electronic form version 1.4