

## Spin Crossover Systems in the Deep Mantle

R. M. Wentzcovitch

*Department of Chemical Engineering and Materials Science,  
University of Minnesota, Minneapolis, MN 55455, USA.*

There has been much interest in spin crossovers found experimentally in the most abundant minerals of Earth's lower mantle ((MgFe)O, (MgFe)(Si,Fe)O<sub>3</sub>-perovskite and post-perovskite) under pressure. Spin crossovers depend strongly on thermodynamic conditions and a full understanding of this problem requires its investigation as function of pressure and temperature. Several aspects of this phenomenon have been difficult to understand based on experiments alone, especially in the perovskite system, and electronic structure calculations are helping to clarify them. The geophysical consequences of these crossovers are yet to be fully understood. I will review progress we have made in understanding spin crossovers and give an overview of this phenomenon and its potential implications for the Earth.

*Research in collaboration with H. Hsu, K. Umemoto, P. Blaha, J. F. Justo, S. de Gironcoli, C. R. S. da Silva, and T. Tsuchiya. Research supported by NSF/ATM-0428774, EAR-0810212, and EAR-1047629, and in part by the MRSEC Program of NSF under Award Number DMR-0212302 and DMR-0819885.*