Abstract Submitted
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Iron spin crossover in the NAL phase and ferromagnesite HAN HSU, National Central University — Spin crossover (SCO) in iron-bearing minerals has attracted tremendous attention, as SCO leads to anomalous changes of the physical properties of these minerals. The local density approximation + self-consistent Hubbard U (LDA+U_{sc}) method, with the U parameters computed self-consistently, has elucidated SCO in many lower-mantle minerals. In this talk, two recent LDA+U_{sc} studies of SCO in earth minerals are presented: the new hexagonal aluminous (NAL) phase [1] and (Mg,Fe)CO_3 ferromagnesite [2]. The former is considered as a main aluminum host in the subducted basalt, and the latter is believed to be the major carbon carrier in the Earth's lower mantle and play a key role in the deep carbon cycle. For both minerals, the abrupt change of iron quadrupole splitting and the volume/elastic anomalies accompanying the SCO obtained in our calculations are in great agreement with experiments. Our calculations also suggest that the spin transition pressure P_T in the NAL phase is not very sensitive to temperature, due to its three nearly degenerate low-spin (LS) states, in contrast with (Mg,Fe)O ferropericlase and (Mg,Fe)CO_3 ferropericlase, in which P_T significantly increases with temperature. [1] H. Hsu, submitted. [2] H. Hsu and S.-C. Huang, Phys. Rev. B **94**, 060404(R) (2016).

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