DFT+*U* investigations of spin crossovers in lower-mantle minerals

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The total electron spin of a transition-metal ion in a crystalline solid can vary with many factors, including temperature, pressure, and strain. This phenomenon, known as spin crossover, is of great technological potential, as it allows artificial control of magnetic properties of materials. Not as widely known, spin crossover may also play a significant role in geophysics. As pressure and temperature increase with depth in the Earth, iron incorporated in minerals can undergo a spin crossover. A well studied example is ferropericlase, the second most abundant mineral in the Earth's lower mantle. In this mineral, a high-spin (HS) to low-spin (LS) crossover occurs in the pressure range of 40-55 GPa, accompanied by elastic, thermodynamic, optical, and conducting anomalies.

In contrast to ferropericlase, spin crossovers in magnesium silicate ($MgSiO_3$) perovskite and post-perovskite, the major mineral phases in the lower mantle, have been controversial for years, due to the complicated nature of these minerals and the difficulty in probing iron spin state directly. Using density functional theory + Hubbard *U* (DFT+*U*) calculations, we investigated spin crossovers in $MgSiO_3$ perovskite and post-perovskite, and our results clarify the iron spin controversy in both mineral phases. We also show that Mössbauer spectroscopy, combined with first-principles calculations, can be a reliable tool to unambiguously identify iron spin state at high pressure [1-4].

[1] Hsu *et al* (2010) *Earth Planet. Sci. Lett.* **294**, 19-26. [2] Hsu *et al* (2011) *Phys. Rev. Lett.* **106**, 118501. [3] Yu *et al* (2012) *Earth Planet. Sci. Lett.* **331-332**, 1-7. [4] Hsu *et al* (2012) *Earth Planet. Sci. Lett.* **359-360**, 34-39.

Meso- to Neo-proterozoic magmatic events and their geological significance: evidences from detrital zircon U-Pb ages of the Jurassic and Cambrian sedimentary rocks in Xishan area, Beijing city, China

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Whether any magmatic records corresponding to the assembly and breaking up of the supercontinent Rodinia are preserved in the North China Craton (NCC) is a key issue to understand the Proterozoic tectonic evolution of the NCC and its correlation to the supercontinent Rodinia. LA-ICP-MS U-Pb dating results of detrital zircons from Jurassic and Cambrian sedimentary rocks in the Xishan area, Beijing city, central part of the NCC show that there are not only ~507 Ma cambrian age peaks, but also ~2.5 Ga, ~2.1 Ga, 1.8-1.66 Ga, ~1.56 Ga, ~1.38 Ga, ~1.14 Ga, ~912 Ma, ~814 Ma, ~740 Ma and ~630 Ma precambrian age records in Cambrian fine sandstone. Also, there are not only ~484 Ma, ~267 Ma, ~241 Ma and ~188 Ma phanerozoic age peaks, but also ~2.77 Ga, ~2.5 Ga, ~2.0 Ga, ~1.78 Ga, ~1.6 Ga, ~1.2 Ga and 848Ma precambrian age records in Jurassic silty mudstone and fine sandstone. Most of Neoarchean and Paleoproterozoic age peaks correspond to significant tectono-magmatic-thermal events previously recognized in the NCC. 1.78-1.38 Ga age peaks correspond to late Paleoproterozoic to Mesoproterozoic multi phase rifting events in the NCC. Zircon ages of 1.3-1.0 Ga and 1.0-0.6 Ga indicate that during the deposition of these sediments there have been significant contributions from 1.3-1.0 Ga and 1.0-0.6 Ga magmatic rocks in the NCC. The magmatic rocks during these periods, which were common in the South China Craton (SCC) and were explained to relate to the assembly and breaking up of the supercontinent Rodinia, were seldom reported in the NCC so far. The finding of 1.3-1.0 Ga and 1.0-0.6 Ga detrital zircons in the NCC may provide clues to understand the possible relationship of the NCC, the SCC and the supercontinent Rodinia.

This work is supported by National Nature Science Foundation of China (Grant No. 41002064) and Special Fund for Basic Scientific Research of Central Colleges, Chang'an University (Grant No. CHD2011JC163).

DOI:10.1180/minmag.2013.077.5.8