The study of hexagonal Fe_2Si

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The tetragonal Fe_2Si in the Pm3-m symmetry group with CsCl structure was found at 1974. Then it was predicted that the compound could be existed on the lunar surface because it has to be formed under space weathering condition. e.g. within airless space or under meteorite impacts. Thereafter, it was indeed found inside a lunar meteorite of a highland-regolith breccia named as Dhofar 280. This kind of tetragonal Fe2Si is called hapkeite.

On the basis of first principle calculations, we showed that a hexagonal structure of Fe_2Si is a ferromagnetic crystal. The result of the phonon spectra indicated that it is a stable structure. Such material exhibits a spin-polarized and half-metal-like band structure. From the calculations of generalized gradient approximation, metallic and semiconducting behaviors, we observed with a direct and nearly 0 eV band gap in various spin channels. The densities of states in the vicinity of the Fermi level were mainly contributed by the *d*-electrons of Fe. We have also calculated the reflection spectrum of Fe_2Si, which had a minima at 275nm and 3300nm with reflectance of 0.27 and 0.49, respectively. The distinct reflection spectra provided a reference for the search of the compound in the future. Such results may provide a reference for the search of hexagonal Fe_2Si in experiments. It is possible that the hexagonal Fe_2Si will symbiont with other Fe-Si compounds under space weathering or meteorite impacts. Whether the hexagonal Fe_2Si exists in the lunar soil, regolith, dust or coexists with other Fe-Si compounds is worthy further study. In addition, we have established a laboratory called "Laboratory of Astrophysics and Astrochemistry" recently. The development of our laboratory follows 3 main directions: 1. To prepare for sample researches of meteorites and Chang'e 5 samples, as which will be the first sample return mission of Chinas; 2. Research on Lunar dust, Martian dust, and solar system evolution; 3 Experiments and simulations of asteroid spectrum. There are some basic equipment in our laboratory: Scanning electron microscope (SEM) with energy dispersive X-ray spectrometry (EDS), Atomic force microscope (AFM), X-Ray diffractometer (XRD), Particle size analyzer, Network analyzer (electrical), UV/Vis NIR Spectrometer and the Dust floating simulation system (which is designed by us). We are looking forward to establish any kind of collaboration with different research groups.